# A graphical calculus for quantum observables

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We present novel laws describing the interaction of a pair of mutually unbiased observables. These laws yield a diagrammatic calculus which enables matrix-free reasoning about quantum systems. To illustrate the elegance of this approach we establish some properties of standard quantum logic gates, compute the quantum Fourier transform and demonstrate equivalence between certain cluster state and quantum circuit computations.

In [1, 2, 8, 11–13] steps were taken towards a diagrammatic formalism to reason about quantum systems. There are several motivations for this development: low level matrix computations are replaced by intuitive topological manipulations of pictures [2]; the algebraic counterpart to these pictures, certain kinds of monoidal categories, support logical reasoning and hence automation [8]; the axiomatic analysis provides insights in which aspects of the quantum mechanical formalism are key to enabling particular quantum phenomena and quantum informatic tasks [1, 11, 13]. In this work we extend such approaches with an archetypal quantum feature: the interaction of incompatible observables.

## ONE OBSERVABLE

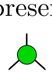
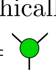
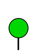
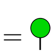
Let $\mathcal{Q}$ be a two-dimensional Hilbert space. Our starting point is the observation in [11] that the linear maps

$$\Delta_Z : \mathcal{Q} \to \mathcal{Q} \otimes \mathcal{Q} :: |i\rangle \mapsto |ii\rangle \qquad \epsilon_Z : \mathcal{Q} \to \mathbb{C} :: |i\rangle \mapsto 1,$$

which respectively *copy* and *delete* the computational base vectors, form a *special †-Frobenius algebra*. The precise definition of this term is not required here: its essential content is contained in Theorem 1. The map $\Delta_Z$ captures the computational base in the following manner: the states $|0\rangle$ and $|1\rangle$ are the only solutions to $\Delta_Z \circ |\psi\rangle = |\psi\rangle \otimes |\psi\rangle$. We will identify the triple $(\mathcal{Q}, \Delta_Z, \epsilon_Z)$ with the spin observable $Z$, whose eigenvectors form this basis. Theorem 1 also involves

$$\Delta_Z^\dagger : \mathcal{Q}\otimes\mathcal{Q} \to \mathcal{Q} :: |ij\rangle \mapsto \delta_{ij}|i\rangle \qquad \epsilon_Z^\dagger : \mathbb{C} \to \mathcal{Q} :: 1 \mapsto \sqrt{2}|+\rangle$$

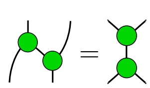
where $\Delta_Z^\dagger$ is known as *fusion* in the quantum computation literature [14, 15]. The maps $\Delta_Z$, $\Delta_Z^\dagger$, $\epsilon_Z$ and $\epsilon_Z^\dagger$ can be represented graphically as [12]

$\Delta_Z =$  $\Delta_Z^\dagger =$  $\epsilon_Z =$  $\epsilon_Z^\dagger =$ 

Reading from the top down, it is immediate that $\Delta_Z$ takes one qubit as input and has two as output; likewise $\epsilon_Z$ has no inputs and one output; the adjoint is represented by flipping a diagram upside down. Composition of maps can be represented by identifying the edges e.g. the *Frobenius identity* [27]

$$(1_\mathcal{Q} \otimes \Delta_Z^\dagger) \circ (\Delta_Z \otimes 1_\mathcal{Q}) = \Delta_Z \circ \Delta_Z^\dagger$$

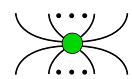
is depicted:



The following holds for any special †-Frobenius algebra [12], hence in particular for the triple $(\mathcal{Q}, \Delta_Z, \epsilon_Z)$.

**Theorem 1.** *Any linear map obtained by composing and tensoring $\Delta_{(Z)}$, $\Delta_{(Z)}^\dagger$, $\epsilon_{(Z)}$, $\epsilon_{(Z)}^\dagger$ and $1_{(\mathcal{Q})}$, and of which the graphical representation is connected, is determined uniquely by the number of inputs and outputs.*

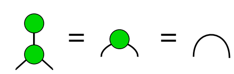
As a consequence, any connected diagram may be represented by a single vertex, keeping the number of inputs and outputs the same, hence the name "spider":



The spider with one input and one output is simply the identity – a line without any vertex. Since we have

$$\Delta_Z \circ \epsilon_Z^\dagger : \mathbb{C} \to \mathcal{Q} \otimes \mathcal{Q} :: 1 \mapsto |00\rangle + |11\rangle\,,$$

we derive the graphical representation of the *Bell state*:



## TWO OBSERVABLES

The basis $\{|+\rangle, |-\rangle\}$ of $\mathcal{Q}$ (and in fact any bases for a Hilbert space [11]) can also be represented by a special †-Frobenius algebra, with

$$\Delta_X : \mathcal{Q} \to \mathcal{Q}\otimes\mathcal{Q} :: |\pm\rangle \mapsto |\pm\pm\rangle \qquad \epsilon_X : \mathcal{Q} \to \mathbb{C} :: |\pm\rangle \mapsto 1,$$

and is also subject to Theorem 1. The *mutually unbiased bases* [18] $(\mathcal{Q}, \Delta_Z, \epsilon_Z)$ and $(\mathcal{Q}, \Delta_X, \epsilon_X)$ stand in a very particular realtionship to each other.

**Proposition 2.** *The quintuple $(\mathcal{Q}, \Delta_Z, \epsilon_Z, \Delta_X, \epsilon_X)$ constitutes a "scaled bialgebra" [28], that is, explicitly,*

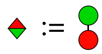
$$\epsilon_Z \circ \epsilon_X^\dagger = \sqrt{2} \tag{1}$$

$$\sqrt{2}\,\Delta_Z \circ \epsilon_X^\dagger = \epsilon_X^\dagger \otimes \epsilon_X^\dagger \qquad \sqrt{2}\,\Delta_X \circ \epsilon_Z^\dagger = \epsilon_Z^\dagger \otimes \epsilon_Z^\dagger \tag{2}$$

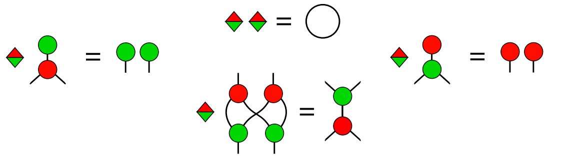
$$\sqrt{2}\,(\Delta_Z^\dagger \otimes \Delta_Z^\dagger) \circ \sigma \circ (\Delta_X \otimes \Delta_X) = \Delta_X^\dagger \circ \Delta_Y \tag{3}$$

*where $\sigma(|ijkl\rangle) = |ikjl\rangle$.*

Note that eq. (2) states that the state determined by $\epsilon_Z^\dagger$ is *clonable up to a scalar* by $\Delta_X$ and vice versa. All these equations are easier to understand in graphical form. We use red dots,  and , for the $X$ structure and retain green for the $Z$. Notice that composing $\epsilon_X \circ \epsilon_Z^\dagger$ is simply the inner product between the corresponding vectors, i.e. $\sqrt{2}$; since this scalar quantity will be frequently required, we introduce a special shorthand symbol:



The laws in Prop. 2 can be written as:

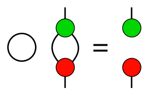


(1)

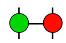
(2)

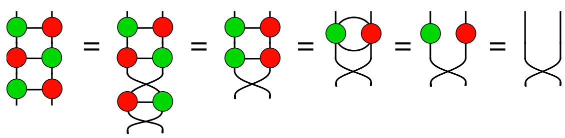
(3)

where the circle in Eq.(1) denotes the *trace* [2] of the identity, which is the dimension of the underlying space. From these we can derive [25]:

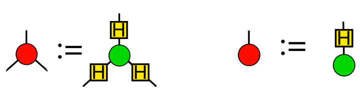


In the interests of clarity the scalar factors will be neglected for the rest of this presentation.

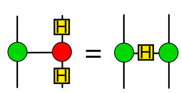
**Example 3.** A quick calculation shows that $(\Delta_Z^\dagger \otimes 1_{\mathcal{Q}}) \circ (1_{\mathcal{Q}} \otimes \Delta_X) = (1_{\mathcal{Q}} \otimes \Delta_X^\dagger) \circ (\Delta_Z \otimes 1_{\mathcal{Q}}) = \wedge X$, hence the controlled-$X$ gate can be represented as  where the red dot is acting on the target qubit. This permits a simple graphical proof of a well known fact:



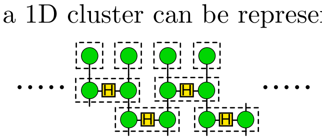
Our language can be augmented with an additional graphical element for the Hadamard gate; $H$ exchanges the $X$ and $Z$ bases, so provides a *colour change rule*:



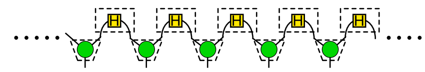

These equations, combined with the fact that $H^2 = 1_{\mathcal{Q}}$, allows not just the changing of one colour into another, but a general transfer principle which states that any "green" concept and its associated equations can be transformed into an equivalent "red" concept obeying the same equations with the colours exchanged. Recall $\wedge Z = (1 \otimes H) \wedge X (1 \otimes H)$; the graphical form shows that this operation is symmetric:



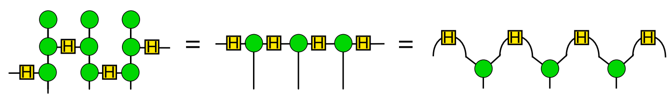
**Example 4.** Cluster states [21], used in measurement-based quantum computing, can be prepared in several ways; the graphical calculus provides short proofs of their equivalence. For example, the original scheme describes a $\wedge Z$ intereaction between qubits initially prepared in the state $|+\rangle$; a 1D cluster can be represented as:



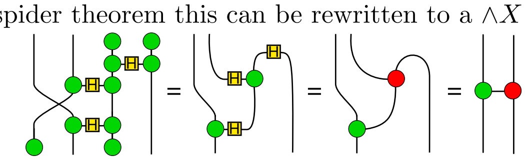
where the boxes delineate the individual $|+\rangle$ preparations and $\wedge Z$ operations. Alternatively, the cluster state can be prepared by fusion of states of the form $|0+\rangle + |1-\rangle$ [15]. Recalling that $\Delta_Z^\dagger$ is the fusion operation, this method of preparation can be represented as [26]:



Again we use dashed lines to indicate the individual components. Using the spider theorem, these are equivalent:

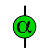
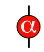


Programs for the one-way model can be verified by translation to an equivalent quantum circuit. E.g. the leftmost diagram below is a post-selected [29] one-way program implementing a $\wedge X$ operation upon its inputs [30]. By the spider theorem this can be rewritten to a $\wedge X$ gate.



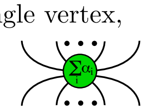
## PHASES

The language we have introduced so far suffices to capture many features of interest in quantum computation, but it cannot yet represent all unitary gates. The remaining necessary primitives are phases. Let

 $= Z_\alpha = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\alpha} \end{pmatrix}$  $= X_\alpha = H Z_\alpha H.$

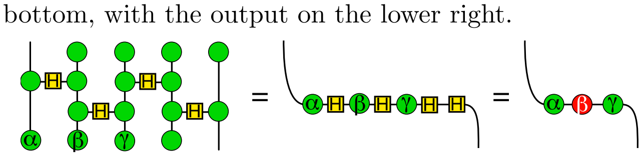
**Theorem 5.** *Any map formed by composition of* $\epsilon_Z$, $\Delta_Z$, $Z_\alpha$, *and their adjoints, whose graphical representation is connected, is uniquely determined by the number of inputs and outputs and the sum, modulo* $2\pi$, *of the* $\alpha$*s which occur on its vertices.*

This generalised spider theorem follows from $Z_\alpha \circ Z_\beta = Z_{\alpha+\beta}$ and $\Delta_Z \circ Z_\alpha = (Z_\alpha \otimes 1_{\mathcal{Q}}) \circ \Delta_Z$. In consequence any diagram consisting only of green vertices may be contracted down to a single vertex,



which is labelled by the sum of all the phases occurring in it. (Of course, the empty green dot corresponds to $\alpha = 0$.) The same holds equally well for the red dots.

**Example 6.** The diagram below shows an implementation of an arbitrary 1-qubit unitary, given as its Euler decomposition $Z_\gamma X_\beta Z_\alpha$ [31]; The input is shown at the top left; this is then bound to the 1D cluster state with a $\wedge Z$ interaction; the four projections are found at the bottom, with the output on the lower right.



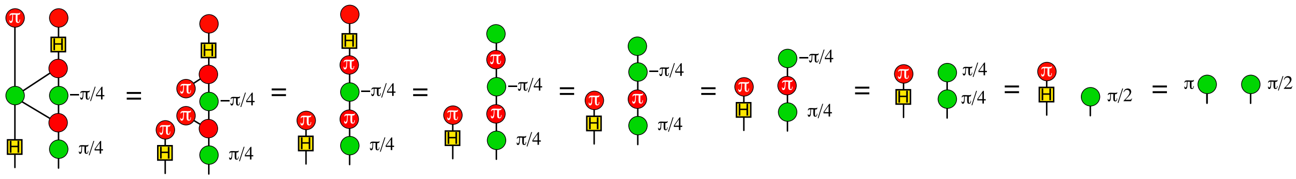



FIG. 1: Graphical simulation of quantum Fourier transform on the input $|10\rangle$.

By simple rewriting steps the implementation is transformed into its specification, i.e. performing an arbitrary 1-qubit unitary, thus proving the program's correctness.

The preceding example uses just green dots because all operations are in the $X-Y$ plane; however there are simple equations governing some interactions between the green $(X-Y)$ operations and the red $(Z-Y)$ operations. Two obvious facts:

$$Z_\alpha |0\rangle = |0\rangle \qquad\qquad Z_\alpha |1\rangle = e^{i\alpha} |1\rangle = |1\rangle$$

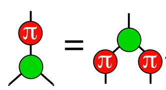
produce simple digrammatic equations:


As before, the same laws hold with the colours exchanged. We will use these laws below.

## NEGATIONS

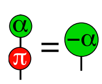
The Pauli $X$ operator exchanges the $Z$-basis vectors $|0\rangle$ and $|1\rangle$; hence $X$ provides a boolean *negation* for the classical structure induced by $\Delta_Z$. As a diagram this is simply $X_\pi =$ . Since $X$ is an operation on the classical data fixed by $\Delta_Z$, we have the equation:

$$\Delta_Z \circ X = (X \otimes X) \circ \Delta_Z$$



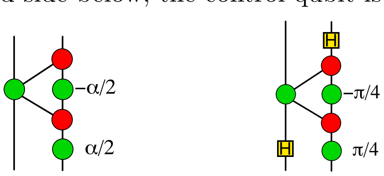

Furthermore, this logical negation induces an *arithmetic* negation on the $X$-phases:

$$X(|0\rangle + e^{i\alpha}|1\rangle) = |1\rangle + e^{i\alpha}|0\rangle = |0\rangle + e^{-i\alpha}|1\rangle$$




The interplay between the logical operations in one basis and the phase information is central to the behaviour of several quantum logic gates.

**Example 7.** We can realise a controlled phase gate, where the phase is an arbitrary angle $\alpha$, as shown on the left hand side below; the control qubit is on the left.




The quantum Fourier transform can be realised as a quantum circuit containing only Hadamard and controlled phase gates; the 2 qubit instantiation of this circuit is shown on the right above. Furthermore, the algorithm can be simulated graphically, as shown in Figure 1.

## DISCUSSION

Our graphical calculus is capable of far more than can be covered in an article of this length. Classical control has not been discussed, but study of control was a motivation for the original axiomatisation of †-Frobenius algebras in [11]. Such notions of control allow the branching behaviour of quantum measurements to be represented. As a consequence, this system subsumes the equational theory of the measurement calculus [22], and can simulate other measurement-based schemes such as logic-gate teleportation [23] and state transfer [24]. Ongoing work aims toward a unified treatment of general measurement-based quantum computing within our graphical setting.

As we have emphasised, the calculus we have described is powerful enough to carry out many computations in the domain of quantum mechanics. However it is known to be *algebraically incomplete*; that is, not every true equation in Hilbert space can be derived graphically. Additional, as yet unknown, axioms will be required to make all desirable equations derivable.

Due to its simple form – the equations are local transformations of undirected graphs – the calculus we have presented is amenable to automation, opening the door to semi- or fully automatic derivation of protocols and algorithms, and proofs of their correctness.

## ACKNOWLEDGEMENTS

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tions of the Foundations III, pages 81–98. AIP Press. arXiv:quant-ph/0510032. The graphical calculus in this paper is presented as a two-dimensional extension of Dirac notation. The fact that (multi-)linear algebraic computations admit a sound and complete graphical calculus traces beck to the work in [3–7].

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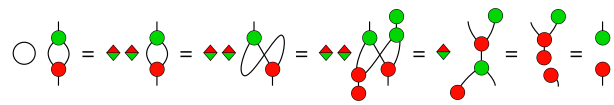
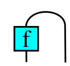
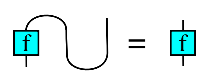
[25] 

[26] Both the Hilbert-Schmidt correspondence for the pure state quantum formalism and Jamiolkowsky correspondence for the mixed state quantum formalism hold in our graphical calculus [1, 2, 13]; given any operation $f$ we obtain the corresponding bipartite state by making $f$ act on a subsystem of a bipartite system in the Bell-state:




Using the spider-theorem we can recover $f$ back by post-composing with the adjoint to the Bell-state:




[27] The reader can verify that this identity indeed holds for $\Delta_Z$ and $\Delta_Z^\dagger$. This remarkable law appeared for the first time in the literature in [16] as part of an axiomatisation of the category of sets and relations.

[28] Our notion of scaled bialgebra differs from the usual notion of bialgebra [19, 20] by the presence of the dimension dependent scalar: all the structural equations of a bialgebra hold, but a scalar factor of $\sqrt{2}$ is introduced. It is easy to show that this bialgebra is a Hopf algebra whose antipode is simply the identity multiplied by 2.

[29] Post-selection allows us to replace measurements with projections onto the +1 eigenstate, simplifying the diagram. However, †-Frobenius algebras were initially introduced in [11] as a formal tool which allows to represent classical control structure so this example can easily be extended with the required unitary corrections.

[30] This implementation is taken from [22].

[31] Like the preceding one, this example is drawn from the measurement calculus [22]; in that syntax it is written $M_1^\alpha M_2^\beta M_3^\gamma M_4 E_{12} E_{23} E_{34} E_{45} N_2 N_3 N_4 N_5$.