

The ZX-calculus is incomplete for quantum mechanics

Christian Schröder de Witt
Scherenbergstr. 22, 10439 Berlin
caschroeder@outlook.com

Vladimir Zamdzhiev
Department of Computer Science
University of Oxford
Oxford, United Kingdom
vladimir.zamdzhiev@cs.ox.ac.uk

We prove that the ZX-calculus is incomplete for quantum mechanics. We suggest the addition of a new 'color-swap' rule, of which currently no analytical formulation is known and which we suspect may be necessary, but not sufficient to make the ZX-calculus complete.

1 Introduction

Coecke and Abramsky pioneered the field of categorical quantum mechanics in [1]. Later, from this study, an intuitive graphical calculus (dubbed the ZX-calculus) was developed by Coecke and Duncan [4][3], which can be used as an alternative to Dirac notation in a wide number of applications [5][11][6][8].

Backens recently proved that the ZX-calculus is complete for an important subset of quantum mechanics, namely stabilizer quantum mechanics, i.e. that for stabilizer quantum mechanics, any equation that can be shown to hold in the Dirac formalism can also be shown to hold within the ZX-calculus[2]. For her proof, she relied on operations on a special class of quantum states, namely graph states. This paper addresses the question of whether the ZX-calculus is complete for the whole of quantum mechanics, and the answer is found to be negative.

1.1 Syntax and Semantics of the ZX-calculus

The syntax and semantics of the ZX-calculus are presented below. The semantics are given in Hilbert space. We begin with atomic diagrams. The inputs to the diagrams are located at the bottom and the outputs are located at the top.

$$\left[\begin{array}{c} | \\ | \end{array} \right] = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I \quad \left[\begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \end{array} \right] = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \sigma$$

$$\begin{aligned}
 \left[\begin{array}{c} \text{cap} \\ \text{cup} \end{array} \right] &= \langle 00| + \langle 11| & \left[\begin{array}{c} \text{cup} \\ \text{cap} \end{array} \right] &= |00\rangle + |11\rangle & \left[\begin{array}{c} \text{H} \\ \text{H} \end{array} \right] &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = H \\
 \left[\begin{array}{c} \text{green dot} \\ \text{fan} \end{array} \right] &= \begin{cases} |0^m\rangle \mapsto |0^n\rangle \\ |1^m\rangle \mapsto e^{i\alpha} |1^n\rangle \\ \text{rest} \mapsto 0 \end{cases} & \left[\begin{array}{c} \text{red dot} \\ \text{fan} \end{array} \right] &= \begin{cases} |+\rangle \mapsto |+\rangle \\ |-\rangle \mapsto e^{i\alpha} |-\rangle \\ \text{rest} \mapsto 0 \end{cases}
 \end{aligned}$$

where in the last two diagrams m is the number of inputs and n is the number of outputs. The labels of the red and green dots form the circle group under addition. So, admissible values are $\alpha \in [0, 2\pi)$. We also make the convention that we will not write a label for the points when $\alpha = 0$.

We can create compound diagrams from smaller diagrams in two ways - either placing two diagrams next to each horizontally, or plugging the outputs of one diagram to the inputs of another. If

$$\left[\begin{array}{c} \Psi_1 \\ \text{fan} \end{array} \right] = D_1 \quad \text{and} \quad \left[\begin{array}{c} \Psi_2 \\ \text{fan} \end{array} \right] = D_2$$

then

$$\left[\begin{array}{c} \Psi_1 \quad \Psi_2 \\ \text{fan} \end{array} \right] = D_1 \otimes D_2$$

and

$$\left[\begin{array}{c} \Psi_1 \\ \Psi_2 \\ \text{fan} \end{array} \right] = D_1 \circ D_2$$

In the latter diagram, the number of outputs of Ψ_2 has to be the same as the number of inputs of Ψ_1 .

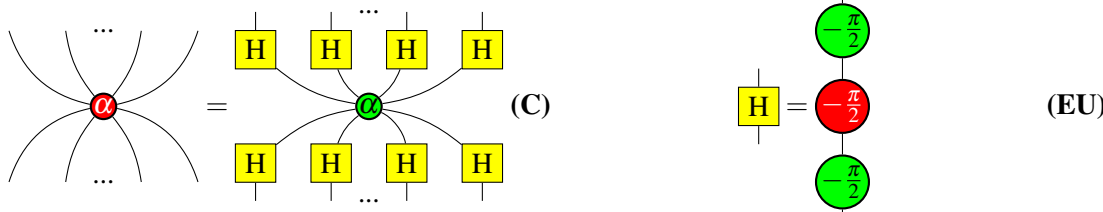
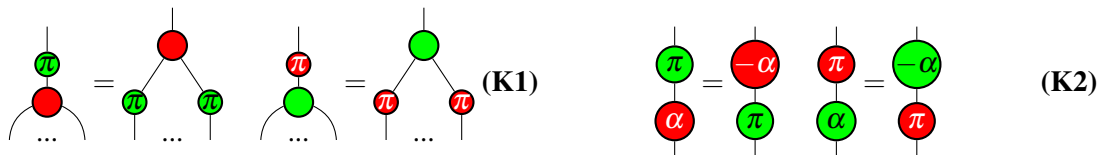
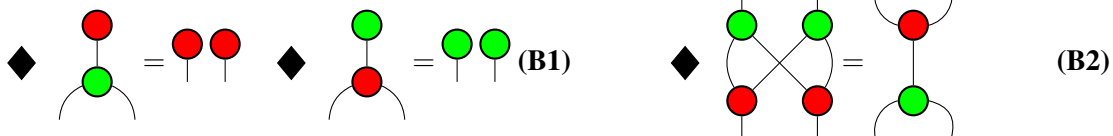
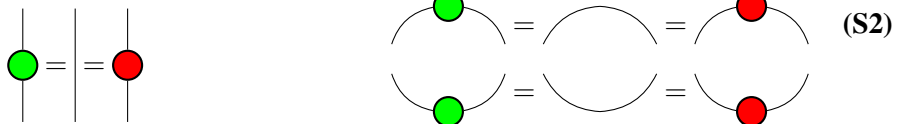
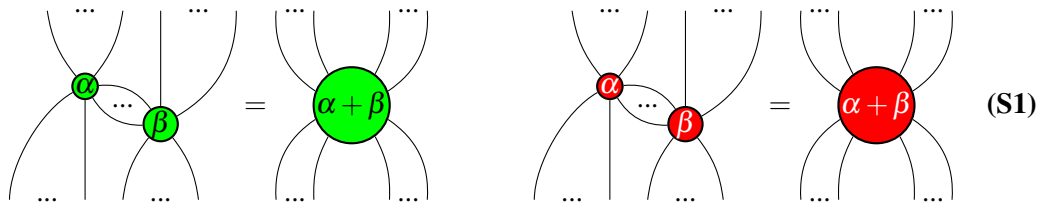
By following the above rules we can represent any pure state map on qubits as a diagram in the ZX-calculus [4].

1.2 ZX Equational Rules

The rules of the ZX-calculus are given by:

"Only the topology matters"

(T)



1.3 Completeness, Soundness and Universality

The original rules of the ZX-calculus, as put forward by Coecke and Duncan [4] did not contain the Euler decomposition of the Hadamard gate, **EU**. Subsequently, Duncan and Perdrix proved [7] that the rule **EU** was not derivable from within the original ZX-calculus. The original ZX-calculus was therefore *incomplete*. Informally, incompleteness signifies that there are equations that can be proven to hold in Dirac-von Neumann notation that cannot be proven in the ZX-calculus. This would reduce the power of the graphical calculus and possibly limit its applications in automated reasoning.

Backens showed in [2] that the current ZX-calculus, which is simply the original ZX-calculus extended by **EU**, is complete for an important fragment of quantum mechanics, namely *stabilizer quantum mechanics (SQM)*. Her proof relies on the fact that each SQM state is, under local Clifford operations [9], equivalent to a special entangled state, namely a *graph state* [10]. This allows one to abstract away from matrix representations and instead decide equivalence between different SQM states by performing *local complementations*, a class of graph manipulations, between graph states. In this way, Backens showed that SQM states may be represented by so-called rGS-LC diagrams, which are only equivalent iff they are graphically identical. In this way, equivalence can be decided in the ZX-calculus.

However, ideally, one would wish the ZX-calculus to be as physically expressive as the complete Dirac-von Neumann formalism. To this goal, three important properties of the calculus need to be established: universality, soundness and completeness.

The ZX-calculus is *sound* [4]. That is, if $ZX \vdash D_1 = D_2$ then $\llbracket D_1 \rrbracket = e^{i\phi} \llbracket D_2 \rrbracket$. In other words, if two diagrams are equal under the axioms of the ZX-calculus, then their Hilbert space interpretations are equal up to a global phase.

Secondly, the ZX-calculus is *universal*, meaning that it can express any quantum state and gate. This is easily proven by showing that the ZX-calculus can express any of the set of universal quantum gates [4].

Finally, *completeness* is the converse of soundness. That is, if $\llbracket D_1 \rrbracket = \llbracket D_2 \rrbracket$ then $ZX \vdash D_1 = D_2$. In the next section, we will show that the ZX-calculus does not have this property.

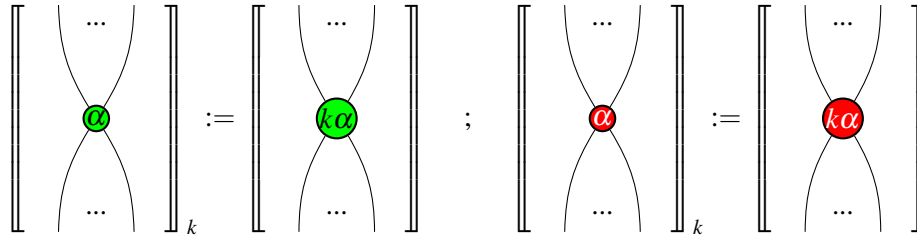
2 Incompleteness

Before we present the proof, let us recall a standard result from quantum mechanics, namely the *Euler decomposition* of single-qubit gates [12]. By this result, any single-qubit unitary gate can be expressed (up to a global phase) through just three consecutive rotations in appropriate bases. For the ZX-calculus, this means that there always exist real angles $\alpha_i, \beta_i, \gamma_i, \phi_i$ such that for any ZX diagram D with one input and one output, we have:

$$\left\| \begin{array}{c} | \\ \hline \boxed{D} \\ \hline | \end{array} \right\| = e^{i\phi_1} \left\| \begin{array}{c} \alpha_1 \\ \beta_1 \\ \gamma_1 \end{array} \right\| = e^{i\phi_2} \left\| \begin{array}{c} \alpha_2 \\ \beta_2 \\ \gamma_2 \end{array} \right\|$$

We prove the incompleteness of the ZX-calculus by using a similar argument to that of Duncan and Perdrix in [7], where they show that the Euler decomposition of the Hadamard gate is not derivable within the ZX-calculus.

In particular, we can define alternative models for the ZX-calculus by setting:

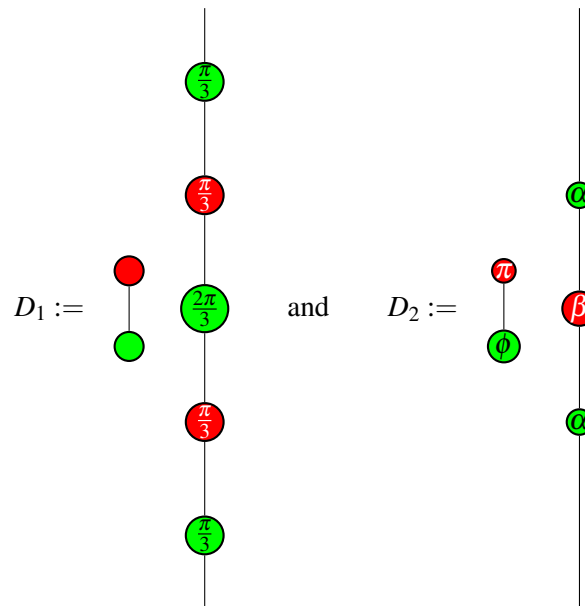


$$[[\cdot]]_k := [[\cdot]], \text{ otherwise}$$

where $k \in \mathbb{Z}$ and $[[\cdot]]$ is the standard interpretation functor for ZX diagrams in Hilbert space. In other words, we multiply all angles in our diagrams by an integer k and consider the corresponding interpretation.

These models are sound when $k = 4p + 1$ for $p \in \mathbb{Z}$. This can be easily verified by checking that each of the equational rules remains valid under this interpretation.

Consider the following two ZX diagrams:



where

$$\begin{aligned}\alpha &:= -\arccos\left(\frac{5}{2\sqrt{13}}\right) \approx 0.2561\pi \\ \beta &:= -2\arcsin\left(\frac{\sqrt{3}}{4}\right) \approx -0.2851\pi \\ \phi &:= \arcsin\left(\frac{\sqrt{3}}{4}\right) - \alpha \approx 0.3987\pi\end{aligned}$$

Then, we have

$$\llbracket D_1 \rrbracket = \llbracket D_2 \rrbracket$$

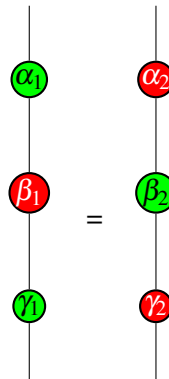
The two scalar factors are introduced so that the equality is exact, otherwise it would be true up to the global phase $e^{i\phi}$.

Let us assume for contradiction that D_1 and D_2 are equal under the axioms of the ZX-calculus, i.e. $ZX \vdash D_1 = D_2$. Since $\llbracket \cdot \rrbracket_{-3}$ provides a sound model of the calculus, it must also be the case that $\llbracket D_1 \rrbracket_{-3} = \lambda \llbracket D_2 \rrbracket_{-3}$, for some $\lambda \in \mathbb{C}$.

However, it is easy to check that this is not true ($\llbracket D_1 \rrbracket_{-3}$ is equal to a scalar times the identity, whereas $\llbracket D_2 \rrbracket_{-3}$ isn't). Therefore the two diagrams D_1 and D_2 are not equal under the axioms of the ZX-calculus, even though they have equal Hilbert space interpretations. This means the ZX-calculus is incomplete.

3 Conclusion and Future Work

The primary contribution of this work is showing that the ZX-calculus is incomplete for quantum mechanics. A natural question to ask is what additional rules can be added to the calculus in order to increase its proving power. The proof that we have used doesn't use any special properties of the presented diagrams – it will be straightforward to apply the same proof to another pair of single-qubit unitary gates where one of them is the Euler decomposition of the other. To eliminate this class of counter-examples, we believe that a "color-swap" rule of the form:

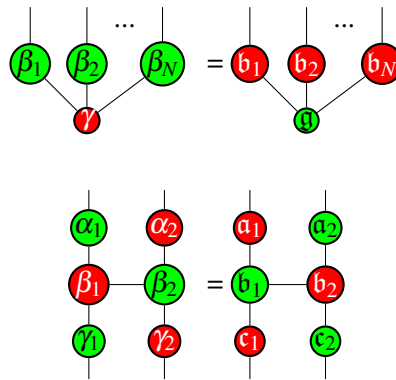


might be needed. This would require identifying functions f_1, f_2, f_3 , s.t. the above rule is valid and

$$\begin{aligned} \alpha_1 &= f_1(\alpha_2, \beta_2, \gamma_2) \\ \beta_1 &= f_2(\alpha_2, \beta_2, \gamma_2) \\ \gamma_1 &= f_3(\alpha_2, \beta_2, \gamma_2) \end{aligned}$$

In other words, an analytic solution for converting from ZXZ to XZX Euler decompositions of single-qubit unitary gates is required.

Whether the addition of such a 'color-swap' would be sufficient to render the ZX-calculus complete is currently unknown. Some simple candidates for further possible non-derivable equalities are presented here:



We suggest to conduct numerical investigations into the question of whether such non-derivable equalities between complex ZX-calculus diagrams exist.

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