The ZH-calculus: completeness and extensions*

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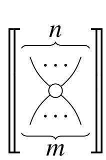
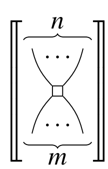
The ZH-calculus is a graphical calculus for describing and manipulating quantum computations, first introduced in [2, QPL'18]. Much like its older cousin, the ZX-calculus [3, 4, 6], it admits straightforward encodings of quantum circuits and several flavours of measurement-based quantum computation (MBQC). However, unlike ZX, ZH is able to elegantly capture and reason about 'AND-gate like' structures (e.g. Toffoli gates) arising in quantum computation.

As a rough analogy with circuits, diagrams of the ZX-calculus can be seen as an extension of the universal families of Clifford+T or Clifford+Rz circuits, whereas ZH-calculus diagrams most readily extend the (also universal [17]) family of Toffoli+Hadamard circuits. This makes them well-suited for producing efficient decompositions of Toffoli gates using *graphical Fourier theory* [13], giving a diagrammatic account of the path-sum approach to quantum circuit verification [20], and working with hypergraph states [14], a generalisation of graph states which feature in several new MBQC schemes [8, 9, 16].

In this article we give a comprehensive account of the core theory of the ZH-calculus, which includes two major new completeness theorems. It was shown in [2] that there exists a complete presentation for ZH if we allow complex-valued parameters. In the current work, we give new completeness proofs for the parameter-free ZH-calculus and a generalisation of the ZH-calculus which takes its parameters from any commutative ring with characteristic $\neq 2$. The result from [2] can therefore be seen as a corollary.

Parameter-free ZH The generators of the parameter-free ZH-calculus—besides the standard identities, swaps, cups and caps—are *Z-spiders*, *H-boxes* and *stars*:


$:= |0\rangle^{\otimes n}\langle 0|^{\otimes m} + |1\rangle^{\otimes n}\langle 1|^{\otimes m}$


$:= \sum(-1)^{i_1\ldots i_m j_1\ldots j_n}\,|j_1\ldots j_n\rangle\langle i_1\ldots i_m|$

$[\![\text{✿}]\!] := \frac{1}{2}$

The sum in the second equation is over all $i_1,\ldots,i_m,j_1,\ldots,j_n \in \{0,1\}$ so that an H-box represents a matrix with all entries equal to 1, except the bottom right element, which is -1.

Using these generators we can define some useful derived generators.


(1)

Parameter-free ZH-diagrams can represent precisely those $2^n \times 2^m$ matrices which are of the form $2^{-k}A$ for some $k \in \mathbb{N}$ and integer matrix A. As shown in Ref. [1] these matrices correspond to those that can be made by the Toffoli+Hadamard gate set (up to some details).

We find that a set of just 8 natural rules suffices to prove completeness for this language:

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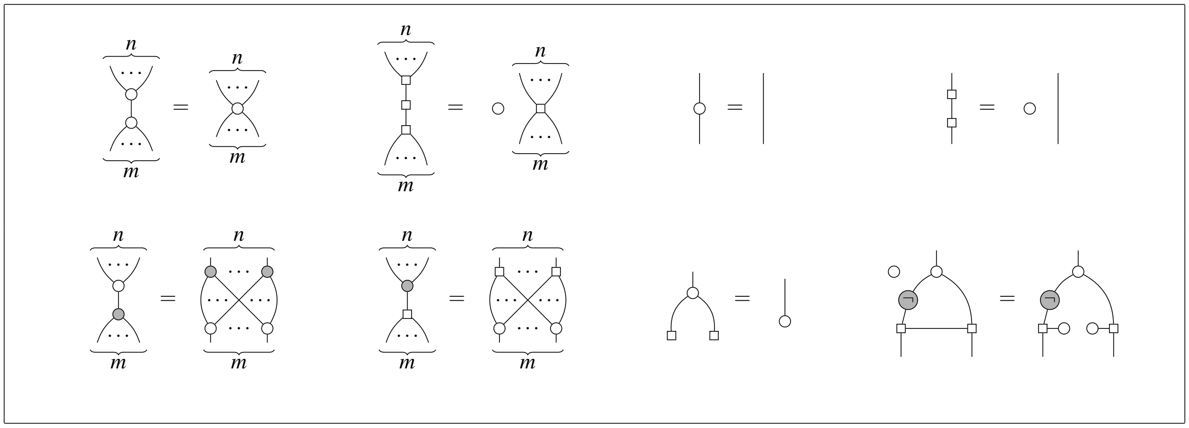
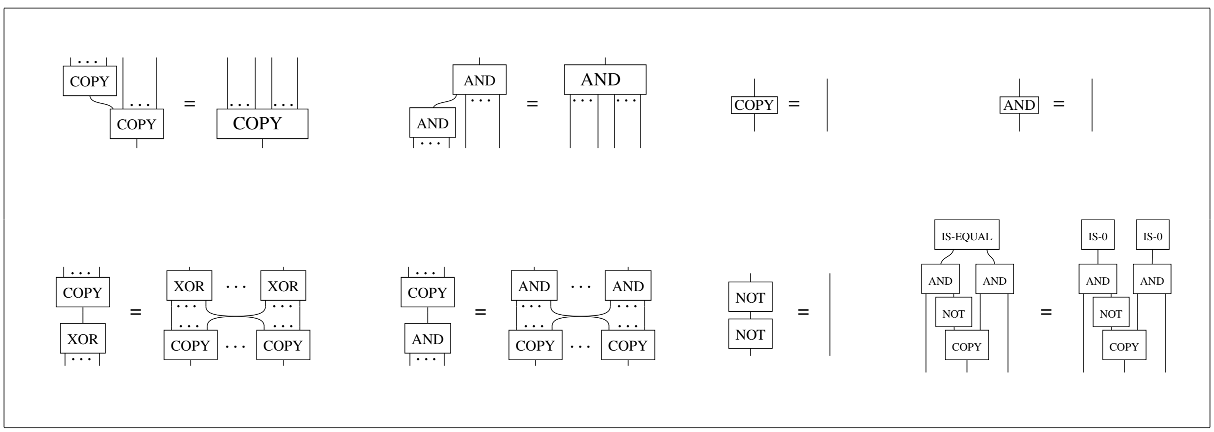
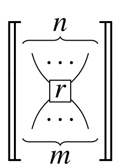


This is significant, because this rule set can be finitely presented and constitutes one of the simplest axiomatisations of a universal family of quantum circuits found to date. Furthermore, each of the rules above, including the less intuitive ‘ortho’ rule on the bottom-right, can be given a direct interpretation in terms of boolean logic:

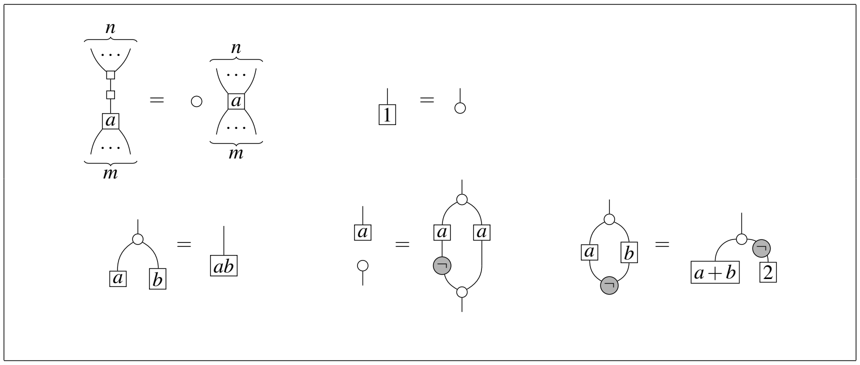


ZH over a ring In the original ZH-calculus of Ref. [2], the H-boxes were labelled by a complex number. We extend this idea and consider a ZH-calculus where the H-boxes are labelled by an element of some chosen ring. Our construction works for any commutative unital ring R where 2 is not a zero-divisor. The construction is different depending on whether 2 is invertible in R or not. In the case where 2 is invertible, i.e. where there is an element $\frac{1}{2}$ in R, the generators of ZH_R are the same as those of parameter-free ZH, except that we define H-boxes labelled by any element $r \in R$:



$$:= \sum r^{i_1 \ldots i_m j_1 \ldots j_n} \left| j_1 \ldots j_n \right\rangle \left\langle i_1 \ldots i_m \right|$$

For $r = -1$ this corresponds to the original H-boxes defined above. The rule set of ZH_R is a superset of the rules presented above for the parameter-free case. The additional rules are:



Here the two rules on the left are generalisations of rules of the parameter-free setting, while the other three rules relate operations of the ring to certain diagrams. We show that our proof of completeness of the parameter-free ZH-calculus extends to this setting, making ZH_R complete over the set of $2^n \times 2^m$ matrices with entries in R.

When $\frac{1}{2} \notin R$ we can still make a complete calculus but we have to be a bit more careful. In particular, we can no longer define the star generator, and hence we cannot define the grey spiders of Eq. (1) as derived generators. Instead, we define the grey spiders as additional generators and relate them to the other generators by employing 'scaled' versions of the definitions (1) as additional rules of the calculus:

Finally, we also need to add a *meta-rule* similar to that of Ref. [12], which tells us that when we have proven an equation of diagrams where on each side there is a scalar Z-spider, then we are allowed to remove this scalar: $\circ D_1 = \circ D_2 \implies D_1 = D_2$.

Previous work A (partial) parameter-free completeness theorem was first claimed in a preprint [22] by a subset of the current authors. However, this earlier result relied on importing a complicated rule which had not previously appeared in ZH and encoding ZH diagrams into another complete graphical calculus, called ZXΔ [19]. The current work supersedes that result by giving a direct proof of parameter-free completeness using a strict subset of the original ZH rules appearing in [2]. Our new proof is interesting also because it shows a direct encoding of the laws of integer arithmetic into the parameter-free ZH-calculus, analogous to the encoding of the rational numbers in the ZW-calculus [7]. Our proof shows directly how each parameter-free ZH-diagram can be reduced to a unique normal form.

Related work The seminal complete graphical language for the fragment of integer matrices is the *ZW-calculus* [5, 10]. This was used as the basis for the first completeness results of the ZX-calculus [11, 15] and resulted in the adding of a new generator, the 'triangle', to some versions of the ZX-calculus in order to represent non-affine Boolean functions. This was later also used to prove completeness over the $\mathbb{Z}[\frac{1}{\sqrt{2}}]$ matrices [19], as well as to find an axiomatisation of the ZX-calculus over arbitrary rings [21]. Compared to these calculi, ours requires less rules, which are smaller, and which are more easily interpretable. The universal ZX-calculus has a rule set that contains fewer rules [18], but one of these rules is a complicated axiom schema requiring iterated trigonometric functions to be specified, while our rule set is entirely finitely presentable.

Conclusion We have found a simple complete axiomatisation of the fragment corresponding to the approximately universal Toffoli+Hadamard gate set. Our proof is entirely self-contained and shows how each diagram can be reduced to normal form. Additionally, we have given an extension of the rule set that gives a complete calculus over an arbitrary commutative ring of characteristic $\neq 2$.

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