Diagrammatic Design of Ansätze for Quantum Chemistry

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Pour ma mère et mon père.
Merci de m'avoir amené jusqu'ici.

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Abstract

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ZxFermion Package

ZxFermion is a Python package built on top of PyZX designed for the manipulation and visualisation of circuits of Pauli gadgets. With built-in Clifford tableau logic using Stim, ZxFermion allows users to quickly implement proofs and test ideas.

VQE algorithms used in quantum chemistry often utilise the UCC framework in which excitation operators have a natural representation as Pauli gadgets. ZxFermion provides a comprehensive toolset designed to be used in a Jupyter notebook environment. Export functionality can be used to generated research paper quality diagrams.

5.1 Creating Gadgets

5.2 Creating Circuits of Gadgets

5.3 Pauli & Clifford Algebra

```
from zxfermion.gates import X, XPlus, XMinus, Z, ZPlus

XPlus + XMinus
>> Identity
```

5.4 Architecture-Aware Circuit Extraction

Appendices

Bibliography

[1] Yordanov, Y. S., Arvidsson-Shukur, D. R. M. & Barnes, C. H. W. Efficient quantum circuits for quantum computational chemistry. *Physical Review A* **102**, 062612 (2020).