

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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Chapter 1

Introduction

1.1 Context & Motivation

Example citation – [1]

1.2 Contribution & Thesis Structure

Chapter 2

Background

2.1 Electronic Structure Theory

2.1.1 The Hartree-Fock Approximation

2.1.2 Coupled-Cluster Theory

2.1.3 Unitary Coupled-Cluster Theory

2.1.4 Hamiltonian Simulation and Trotterisation

2.1.5 Fermionic-Qubit Encodings

Jordan-Wigner Transformation

Bravyi-Kitaev Transformation

Parity Mapping

2.2 The ZX Calculus

2.2.1 Generators

2.2.2 Rewrite Rules

Chapter 3

Variational Quantum Algorithms

3.1 Variational Quantum Algorithms

Chapter 4

Phase Polynomials

4.1 Phase Gadgets

4.1.1 Algebraic Structure

4.1.2 ZX Calculus Representation

4.1.3 Phase Gadget Decomposition

4.2 Pauli Gadgets

4.3 Controlled Rotations

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).