

# 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).