Автономная некоммерческая
образовательная организация высшего образования
«Сколковский институт науки и технологий»

На правах рукописи

Биамонте Джейкоб Дэниел

О МАТЕМАТИЧЕСКОЙ СТРУКТУРЕ МОДЕЛЕЙ КВАНТОВЫХ ВЫЧИСЛЕНИЙ НА ОСНОВЕ МИНИМИЗАЦИИ ГАМИЛЬТОНИАНА

01.01.03– математическая физика

АВТОРЕФЕРАТ

диссертации на соискание ученой степени

доктора физико-математических наук

МОСКВА – 2021

Работа выполнена в Автономной некоммерческой образовательной организации высшего образования «Сколковский институт науки и технологий».

Ведущая организация : Федеральное Государственное Бюджетное Образовательное Учреждение Высшего Образования "Московский государственный университет имени М.В.Ломоносова"

Защита диссертации состоится 29 апреля 2022 г. в 14-00 на заседании диссертационного совета ФПМИ. 01.01.03.001 по адресу: 141701, Московская область, г. Долгопрудный, Институтский переулок, д. 9.

С диссертацией можно ознакомиться на сайте Московского физико-технического института (национального исследовательского университета)
https://mipt.ru/education/post-graduate/soiskateli-fiziko-matematicheskie-nauki.php

Работа представлена «04» октября 2021 г. в Аттестационную комиссию федерального государственного автономного образовательного учреждения высшего образования «Московский физико-технический институт (национальный исследовательский университет)» для рассмотрения советом по защите диссертаций на соискание ученой степени кандидата наук, доктора наук в соответствии с п. 3.1 ст. 4 Федерального закона «О науке и государственной научно-технической политике».

Ученый секретарь
диссертационного совета
ФПМИ.01.01.03.001,
к.т.н., доцент Войтиков К.Ю.

Autonomous non-profit organization for higher education
SKOLKOVO INSTITUTE OF SCIENCE AND TECHNOLOGY

© manuscript author's signature

Jacob Daniel Biamonte

ON THE MATHEMATICAL STRUCTURE OF QUANTUM MODELS OF COMPUTATION BASED ON HAMILTONIAN MINIMISATION

01.01.03 - Mathematical Physics

Synopsis of the

Dissertation submitted for the degree of

Doctor of Physical and Mathematical Sciences

Moscow — 2021

The dissertation was completed at the autonomous non-profit organization for higher education “Skolkovo Institute of Science and Technology”

Leading Organization -Federal State Budgetary Educational Institution of Higher Education ”Lomonosov Moscow State University”

The defense will take place on 29 April 2022 at 14:00 at the meeting of the dissertation council FPMI.01.01.03.001 in 141701, Moscow region, Dolgoprudny, Institutskiy pereulok, 9.

The dissertation can be found on the website of Moscow Institute for Physics and Technology (National Research University)
https://mipt.ru/education/post-graduate/soiskateli-fiziko-matematicheskie-nauki.php

The dissertation was sent to the certifying commission of the Federal state autonomous organization for higher education Moscow Institute for Physics and Technology (National Research University) for review for the degree of the Doctor of Physical and Mathematical Sciences in accordance with clause 3.1 of article 4 of the Federal law “On science and state scientific and technical policy” on October 4, 2021.

Scientific Secretary
Dissertation council
FPMI.01.01.03.001,
Ph.D., Associate Professor Voytikov K.Yu.

GENERAL TOPICAL CHARACTERIZATION

This dissertation develops the mathematical apparatus and considers problems surrounding models of quantum (and classical) computation that minimize Hamiltonians.

Over the last 100 years, quantum effects have played increasingly prevalent roles in technology. The period ranging from the dawn of the transistor and the advent of the laser up until today is referred to as 'the first quantum revolution.' The first quantum revolution utilized collective (a.k.a. average or mean field) quantum effects. We are now entering the 'second quantum revolution.' Bootstrapping precision instruments and the dramatic technological developments pioneered in the first quantum revolution, humankind is increasingly able to control the quantum states of individual and interacting particles. At this scale, matter provides phenomena that lead to new possibilities to store and manipulate (quantum) information.

The study of quantum mechanics is deeply rooted in traditional Russian science and underpins part of the countries mathematical physics tradition. Indeed, the foundations of the first quantum revolution finds a long list of pioneers, from the great Nikolay Bogolyubov to the somewhat lesser known Ludvig Faddeev and Vladimir Fock. From the onset Russian scientists produced several extremely important early results which paved the way for the second quantum revolution. Everyone in the Western world knows well that in the early 1980s Richard Feynman conjectured that a quantum computer had the potential to simulate physical processes that a classical computer could not [International Journal of Theoretical Physics, 21(6-7):467 (1982)]. It is however lesser known in the West that Yuri Manin independently conjectured the inherent computational power of quantum mechanics [Vychislimoe i nevychislimoe (English: Computable and uncomputable), Soviet Radio, (1980)].

Alexander Holevo's 1973 bound, which establishes an upper bound to the amount of information that can be known about a quantum state (accessible information) is perhaps more widely known outside of Russia [Problems of Information Transmission, 9(3):177 (1973)]. And of course Boris Tsirelson's 1980 work towards an upper limit to quantum mechanical correlations between distant events

is again widely known today [Letters in Mathematical Physics, 4(2):93 (1980)]. As far as laying the foundations of quantum computation and quantum computational complexity theory, Alexei Kitaev made extraordinary developments. Several of Kitaev's results defining quantum complexity classes (through the so called, Local Hamiltonian problem), creating Hamiltonian gadgets and introducing the phase estimation algorithm underpin several of the chapters in this work.

Recent developments in quantum information processing have fostered a global research effort to understand and develop applications for noisy real-world quantum information processors (often called NISQ: Noisy Intermediate-Scale Quantum (NISQ). Unlike traditional textbook quantum algorithms, quantum algorithms executed on NISQ devices operate in the presence of systematic and random errors. In practice this limits the depth of the circuit that can be executed. Experimental developments have lead to a novel utilitarian means of quantum computation enabled by an iterative classical-to-quantum feedback process called, variational quantum computation. Variational quantum computation arrives after ample progress in ground state quantum computation by quantum annealing.

Questions related to quantum programming are no longer isolated to a small community (as was the case until just a few years ago). The topic of quantum algorithms and quantum applications has rapidly transformed from a small academic theoretical community to one driven by major technology leaders and backed by ample private and public investment. Dedicated programs have been initiated around the globe devoted to solve these questions. This dissertation focuses on the development of the mathematical framework and the use of mathematical tools needed to address these challenges. The central theme of Hamiltonian ground states provides several additional fruitful connections to areas of growing interest in mathematical physics.

DISSERTATION GOALS

We aim to present a consistent and general framework, which conceptually binds many of the tools used across contemporary quantum programming. The unifying focus is on properties of ground states of Hamiltonians. Programming ground states is required in adiabatic quantum computation and other models of ground state annealing while Hamiltonian minimization is also central to physics and chemistry simulation algorithms that are widely anticipated future quantum computing applications.

The goal is then simply stated. We present a coherent view that develops mathematical structures and connects the core ideas across the areas of:

(i) Ground state and adiabatic quantum computation.

(ii) The quantum simulation of ground state properties of physical systems.

(iii) The variational approach to effective Hamiltonian minimization.

Indeed, the variational model of quantum computation is stated by means of a Hamiltonian minimization problem that utilizes a classical-to-quantum feedback loop. We further model and formalize this algorithmic process.

RESEARCH METHODS AND METHODOLOGY

Methods from the theory of algebraic and strongly order structures (graded algebras), matrix analysis, elementary group theory and algebraic graph theory where used. Additional techniques include Boolean algebras, and Green's function based perturbation theory as well as computational complexity theory. The mathematical structure of quantum mechanics was further relied on.

MAIN STATEMENTS DEFENDED

1. The formulation of the Ising and quantum kernel problem statements and development of a mathematical apparatus to program parent Hamiltonian models with specific ground state properties.
2. The development of specific and improved k-body to 2-body Hamiltonian reductions.
3. Proof that the von Neumann entropy of stochastic propagators on a graph is subadditive.
4. Showing that (i) $|y_+\rangle = |0\rangle + i|1\rangle$, (ii, iii) cups and caps, (iv) Hadamard and (v) COPY generate any Clifford tensor network and hence that the ZX tensor rewrite system admits a poly-time terminating rewrite sequence establishing the Gottesman–Knill theorem.
5. The combinatorial quantum circuit area law bounds the maximum possible entanglement across any bipartition of qubits acted on by a quantum circuit comprised of local unitaries and CNOT gates.
6. Utilization of the parent Hamiltonian mathematical apparatus and gadgets to embed quantum and classical circuits into the low energy sector of Hamiltonians, thereby contributing mappings of **MA**- and **QMA**-hard problem instances to **MA**- and **QMA**-hard Hamiltonian ground state energy decision problems.
7. Utilization of the mathematical apparatus to embed quantum and classical circuits into the lowest energy state of Hamiltonians thereby mapping **MA**- and **QMA**-hard problem instances to **MA**- and **QMA**-hard Hamiltonian ground state energy decision problems.
8. Proving that physically relevant Hamiltonians—including the tunable Ising model with additional XX-interactions—can embed universal quantum computational resources for ground state quantum computation.
9. The development of the mathematical model to describe variational quantum computation and the establishment of the computational universality of the *variational model of quantum computation*.

SCIENTIFIC NOVELTY

The primary results defended in this dissertation have appeared in peer reviewed journals. I hope the dissertation itself culminates to produce an emergent type of novelty for its readers!

We devised a structured (ordered) algebraic approach to understand quantum states and to derive and engineer properties of generalized Ising Hamiltonian penalty functions. Penalty functions were developed to embed logic operations (gates) into the low-energy sector of Ising spins. Likewise, three (and higher) body interaction Ising terms were mimicked through the minimisation of 2- and 1-body Ising terms.

We contrast stochastic and quantum mechanics through the language of walks on graphs. Any finite dimensional quantum (or stochastic) process can be viewed as a walk on the graph defined by the support of its generators. This framework aids in understanding the differences between quantum and stochastic mechanics by better defining the mathematical similarities and differences of the theories. For example, this enabled the development of a spectral graph function which provably satisfies both (i) the definition of an entropy and (ii) subadditivity.

By a merger of techniques appearing in the theory of tensor networks, categorical quantum mechanics and Boolean circuit theory, we employ a tensor network/quantum circuit variant which corresponds to the known ZX graphical calculus. We recall simplistic generators for the class of Clifford tensor networks. We further use this system to recover the Gottesman–Knill theorem by graphical rewrites.

Using ideas related to the area law in tensor network theory, we develop a combinatorial quantum circuit area law. This bounds the maximum possible entanglement across any bipartion of qubits acted on by a quantum circuit comprised of local unitaries and CNOT gates. It has practical significance in that it provides a lowerbound on the depth of circuits needed to maximize bipartite entanglement across all possible partitions.

Using ideas from the theory of computational phase transitions, particularly those found in 3-SAT, we studied the performance of the quantum approximate optimization algorithm. We found and quantified how increasing a problems con-

straint to variable ratio can induce under parameterization and cause quantum approximate optimization (QAOA) algorithms to fail.

Building ideas from Hamiltonian complexity theory, the contemporary variational approach to quantum-enhanced algorithms was proven to enable a universal model of quantum computation. Hence, any quantum algorithm can in principle be executed as a variational algorithm.

By considering infinite series and tailoring them to cancel errors, several constructions related to Hamiltonian gadgets are improved. These and other techniques are used to prove that physically relevant two-body model Hamiltonians have QMA-complete ground state energy decision problems. They hence provide a universal resource for ground state quantum computation.

PRACTICAL AND THEORETICAL SIGNIFICANCE

The practical significance of this work is justified due to this rapid increase in experimental demonstrations of quantum information processing. Indeed, there is now a global effort to understand the computational capacity and the scope of applications possible on NISQ-era quantum processors. Recent state of the art demonstrations include the following:

1. QAOA. The Google team has used transmon qubits to show QAOA results for up to 17 qubits with depth-3 ansatz levels [Nature Physics 17, 332-336 (2021)]. As the authors scaled the number of qubits to produce their dataplot, we believe that they avoided reachability deficits. A numerical study that places their findings as a cross section of a larger analysis will show the region of their instances, which appear to be statistically representative.
2. VQE (chemistry). The Google team has used transmon qubits to show a VQE approach to create a Hartree-Fock approximation to the ground state of hydrogen chains using 12 qubits in [Science 369 (6507), 1084 (2020)]. Their ansatz was of modified checkerboard form.
3. VQE (lattice simulation). Self-verifying variational algorithms as proposed in [Nature 569, 355 (2019)] and elsewhere have vanishing objec-

Experiment	Organization	Qubits	Ansatz	Depth	year
Ising model	Cornell/IBM	20	Alternating	25	2021
QAOA	Google	23	Split operator	4	2021
High energy model	MSU/SkT	2	Checkerboard	3	2021
Supremacy	Google	53	HEA	20	2019
Lattice model	Innsbruck	20	Split operator	6	2019
Chemistry	IBM	6	HEA	2	2017

Table 1 — Justification of the qubit model in terms of ansatz demonstrations of specified depth/qubit counts.

tive functions when the solution is reached. Such an approach was used in [Nature 569, 355 (2019)] to simulate the ground state of the lattice Schwinger model using 8 qubits realized by trapped ions.

While there is a practical outlet for these results, development of the theory and foundations of the subject is centrally aligned with the present dissertation. For example, by presenting a new provably universal model of quantum computation, the thesis elevates the standing of variational quantum computation to the same standing as the other universal models. The dissertation also presents several new tools. For instance, new gadget constructions are given, showing for example that YY terms can be emulated (low energy effective Hamiltonian) using only Z, ZZ and XX.

CONSISTENCY OF RESULTS

This thesis considers qubits. For short (non-error corrected) circuits this model is physically justified as follows (see the experimental summary in Table 1):

1. NISQ Era variational quantum algorithms consider a fixed error tolerance and tune a short quantum circuit to minimize an objective function.
2. Circuits with dozens of gates can now be realized with negligible accumulated total error:

The validity of the results are confirmed by consistency with prior art and rigorous mathematical proofs wherever appropriate. Numerical experiments were sometimes also employed which reconfirm analytical findings.

Results forming this dissertation date back several years and appeared in peer reviewed journal articles. Several of these results now comprise parts of the accepted literature on the topic. This includes work on Ising model embeddings, work on stochastic versus quantum walks, developing more general perturbation gadgets as well as results on using phase estimation for quantum simulation.

This so-called *variational* approach to quantum computation was formally proven (in the noise free setting) to represent a universal model of quantum computation by this thesis. This extended and built on several known results appearing in the related topic of Hamiltonian complexity theory. Many recent studies have not quantified the number of terms needed in the penalty function to implement a variational algorithm. We hence define a cardinality measure and quantify the number of Pauli terms in the sigma basis. This is consistent with past findings but presents a new focus to quantify penalty functions.

In addition, many studies have presented various penalty functions to illustrate that variational algorithms are capable of algorithmic tasks. A universality proof shows that penalty functions in principle are more general. This is again consistent with the state of the art. The original published papers which present these results have become accepted parts of the literature, some over a decade old.

PRESENTATION OF THE RESULTS

Contents and results from this dissertation were presented by the author to peers as follows (talks entirely dedicated to the presentation of the DSc thesis are denoted with '[Thesis presentation]' preceding the title of the thesis):

1. **[Thesis presentation] On the mathematical structure of quantum models of computation based on Hamiltonian minimisation**
   I.E. Tamm Theory Department, P.N. Lebedev Institute of Physics, the

Russian Academy of Sciences, Moscow, Russian Federation, 22 September 2021

2. [**Thesis presentation**] **On the mathematical structure of quantum models of computation based on Hamiltonian minimisation** Laboratory of Quantum Optics and Quantum Information, Center for Advanced Studies, Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russian Federation, 15 September 2021
3. [**Thesis presentation**] **On the mathematical structure of quantum models of computation based on Hamiltonian minimisation** Department of Supercomputers and Quantum Informatics, The Faculty of Computational Mathematics and Cybernetics, Lomonosov Moscow State University, Moscow, Russian Federation, 14 September 2021
4. [**Thesis presentation**] **On the mathematical structure of quantum models of computation based on Hamiltonian minimisation** Department of Higher Mathematics, Moscow Institute of Physics and Technology, Moscow, Russian Federation, 8 September 2021
5. [**Thesis presentation**] **On the mathematical structure of quantum models of computation based on Hamiltonian minimisation** Skolkovo Institute of Science and Technology, Moscow, Russian Federation, 7 September 2021
6. [**Thesis presentation**] **On the mathematical structure of quantum models of computation based on Hamiltonian minimisation** Kazan Quantum Center, Kazan National Research Technical University named after A.N. Tupolev, Kazan, Russian Federation, 4 September 2021
7. [**Thesis presentation**] **On the mathematical structure of quantum models of computation based on Hamiltonian minimisation** Max Planck Institute of Quantum Optics, Hans-Kopfermann-Str. 1 85748 Garching, 21 July 2021
8. **On variational quantum computation** (General Institutional Seminar), P.N. Lebedev Institute of Physics, the Russian Academy of Sciences, Moscow, Russian Federation, 17 March 2021
9. [**Thesis presentation**] **On quantum computation by variation of a quantum circuits parameters to minimise an effective Hamil-**

tonian iteratively realised by local measurements
Department of Mathematical Methods for Quantum Technologies, Steklov Mathematical Institute of the Russian Academy of Sciences, Moscow, Russian Federation, 25 March 2021

10. [**Thesis presentation**] **On the mathematical structure of quantum models of computation based on Hamiltonian minimisation**
Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation, 25 September 2020
11. [**Thesis presentation**] **On the mathematical structure of quantum models of computation based on Hamiltonian minimisation**
The Russian Quantum Center, Skolkovo, Russian Federation, 26 Aug 2020
12. [**Thesis presentation**] **On the mathematical structure of quantum models of computation based on Hamiltonian minimisation**
M.V. Lomonosov Moscow State University Quantum Technologies Center, Moscow, Russian Federation, 14 July 2020
13. **Variational Models of Quantum Computation**
Episode IX, Google Research Series on Quantum Computing
Google Poland, Warsaw Poland, 10 October 2019
14. **A Universal Model of Variational Quantum Computation**
Quantum Machine Learning and Data Analytics Workshop
Purdue University, Discovery Park, West Lafayette Indiana
United States, September 2019
15. **Quantum Enhanced Machine Learning**
Physics Challenges in Machine Learning for Network Science
Queen Mary University of London
London, United Kingdom, September 2019
16. **Quantum Machine Learning for Quantum Simulation**
Machine Learning for Quantum Matter
Nodita, Stockholm, Sweden, August 2019
17. **Recent Results in the Theory of Variational Quantum Computation**
the 5th International Conference on Quantum Technologies
The Russian Quantum Center, Moscow Russia 2019

18. **Variational Quantum Computation in Photonics**
    The 28th Annual International Laser Physics Workshop
    Gyeongju, South Korea, July 2019
19. **Trends in Variational Quantum Algorithms**
    Overview style talk given (multiple times) at
    (a) Riken Institute (Japan)
    (b) NTT laboratories (Tokyo, Japan)
    (c) CIIRC Institute (Prague)
20. **Quantum Machine Learning Matrix Product States**
    Keynote talk at the Workshop on Quantum Information
    Harvard, USA, April 23-24, 2018
21. **Quantum Complex Networks**
    Keynote Lighting Talk at International school and conference on network science (NetSci)
    Paris, France 2018

PUBLICATIONS

The author has 62 papers listed in Scopus [September 2021]. The thesis compiles results from 20 primary research articles, 1 book and two review articles. A list of 20 publications is given at the end of this synopsis.

AUTHOR CONTRIBUTION

The author has had many successful collaborations. The main results of the dissertation were published in small teams or as single author manuscripts. Results derived with collaborators are clearly indicated as such, either in the body of the text or in reference to the result/theorem. The focus has been on the authors own contribution to these joint works.

DISSERTATION STRUCTURE

The dissertation consists of an introduction, 6 chapters, a conclusion, a list of symbols, a list of abbreviations, a glossary of terms, a bibliography, a list of figures, a list of tables and finally an alphabetical index.

DISSERTATION CONTENTS

To present the most central portions of the theory underpinning contemporary quantum algorithms, we focus on Hamiltonian ground states. The rudimentary though still non-trivial starting point is understanding how to program ground states of Ising type models.

We state the following properties of quantum theory stated in terms of quantum bits (qubits).

Definition 1 (Complex Euclidean space)**.**

$$V_n = [\mathbb{C}^2]^{\otimes n} \cong [\mathbb{C}]^{2^n} \tag{1}$$

We will equivalently write $[\mathbb{C}^2]^{\otimes n}$, $\mathbb{C}_2^{\otimes n}$.

Remark 1. $\mathcal{L}(\mathbb{C}_2^{\otimes n})$ denotes the space of linear maps from $\mathbb{C}_2^{\otimes n}$ to itself.

The dissertation considers the following linear maps:

Remark 2 (Linear qubit maps)**.**

1. States: $\psi \in V_n$
2. Effects: $\psi^\dagger \in V_n^\star = (V_n \to \mathbb{C})$.
3. Hamiltonians A in $\text{herm}_{\mathbb{C}}(2^n) \equiv \{A \in \mathcal{L}(V_n) \mid A = A^\dagger\}$.
4. Propagators U in $\mathbf{U}_{\mathbb{C}}(2^n) \equiv \ \{U \in \mathcal{L}(V_n) \mid U^\dagger U = \mathbb{1}\}$.

Remark 3 (Inner product)**.** The standard inner product is used:

$$\langle \cdot | \cdot \rangle : V_n^* \otimes V_n \to \mathbb{C}, \ \ (\phi,\psi) \to \langle \phi | \, \psi \rangle = \sum_j \bar{\phi}_j \psi^j \in \mathbb{C}.$$

States/effects are unit ℓ_2 vectors.

Remark 4 (Computational basis)**.** The dissertation tends to fix the so called, computational basis:

1. n-qubit basis: $\mathcal{B}_n = \{|0\rangle, |1\rangle\}^{\otimes n}$ with 2^n orthonormal basis vectors
2. Single qubit basis: $|0\rangle, |1\rangle \in \mathcal{B}_1$
3. $\text{span}_{\mathbb{C}}\{\mathcal{B}_n\} \cong V_n = [\mathbb{C}^2]^{\otimes n}$

Remark 5 (Properties of Sigma matrices)**.** This thesis makes use of the following properties of Sigma matrices:

1. $\sigma^l \sigma^m = \imath \varepsilon_{lmn} \sigma^n + \delta_{lm} \mathbb{1}$
2. $R_{\boldsymbol{n}}(\theta) = e^{-\imath\theta(\boldsymbol{n}.\boldsymbol{\sigma})} = \cos\theta - \imath(\boldsymbol{n}.\boldsymbol{\sigma})\sin\theta$, where $\boldsymbol{n}.\boldsymbol{\sigma} \equiv n_1\sigma^1 + n_2\sigma^2 + n_3\sigma^3$
3. $\text{herm}_{\mathbb{C}}(2^n) = \text{span}_{\mathbb{R}}\left\{\bigotimes_{l=1}^n \sigma_l^{\alpha_l} \mid \alpha_l = 0,1,2,3\right\}$
4. $\sigma_k^a \equiv \mathbb{1}_1 \otimes \ldots \otimes \mathbb{1}_{k-1} \otimes \sigma_k^a \otimes \mathbb{1}_{k+1} \otimes \ldots \otimes \mathbb{1}_n$

Definition 2 (Pauli group)**.** $\mathbf{P}_n = \left\{e^{\imath\theta\pi/2} \bigotimes_{j=1}^n \sigma^{\alpha_j} \mid \theta, \alpha_j = 0,1,2,3\right\}$.

Remark 6. $\text{span}\{\text{Re}(\ \mathbf{P}_n)\} = \text{span}_{\mathbb{R}}\left\{\bigotimes_{l=1}^n \sigma_l^{\alpha_l} \mid \alpha_l = 0,1,2,3\right\}$.

Definition 3 (Clifford group)**.** $\mathbf{C}_n = \{C \in \mathbf{U}(2^n) \mid C\mathbf{P}_n C^\dagger = \mathbf{P}_n\}$.

Remark 7. For $C \in \mathbf{C}_n$,

$$C\left(\bigotimes_{j=1}^n \sigma^{\alpha_j}\right)C^\dagger = \pm\bigotimes_{j=1}^n \sigma^{\gamma_j} \tag{2}$$

for $\alpha_j, \gamma_j \in \{0,1,2,3\}$.

Remark 8 (The expected value of a Hamiltonian relative a state)**.** The dissertation will consider the expected value as:

$$(A, \psi, \psi^\dagger) \to \langle\psi| A |\psi\rangle = \sum_{l,m} A_{l,m}\bar{\psi}_m\psi_l \in \mathbb{C}$$

for $A \in \text{herm}_{\mathbb{C}}(2^n)$.

The dissertation works with Hamiltonian operators. The simplest case is the generalized Ising model.

Remark 9 (Generalized Ising model)**.** A generalized Ising model is an energy function of a symmetric graph $G = (E, V)$. The energy (Hamiltonian) function is given as:

$$H_{\text{Ising}} = \sum_{j \in V} h_j s_j + \frac{1}{2} \sum_{l,m \in E} J_{lm} s_l s_m. \tag{3}$$

where $s_j \in \{\pm 1\}$

The dissertation relies on connections between problems in mathematical physics and the theory of complexity.

Remark 10. We assume all numbers are defined to some fixed but arbitrary finite precision to avoid pathologies.

Definition 4 (The class **NP**)**.** A problem class Γ is said to be inside **NP** if candidate solutions to instances $\omega \in \Gamma$ can be verified in time $\mathcal{O}(\text{poly}(|\omega|))$.

The concept of minimisation problems where the inputs are *easy* to evaluate is one of the concepts motivating the dissertation. For example: one can determine the energy of a given spin configuration with respect to the following Hamiltonian using an algorithm that is polynomial in the number of Hamiltonian terms/size of the input.

$$H_{\text{Ising}} = \sum_{i} h_i s_i + \sum_{i,j} J_{ij} s_i s_j. \tag{4}$$

Remark 11. The minimisation of generalized Ising Hamiltonians is **NP**-hard.

Definition 5. A problem is **NP**-hard if all problems inside **NP** can be reduced to it (Karp reduction).

Definition 6. A problem is **NP**-complete when it is in **NP** and also **NP**-hard.

Definition 7. A language $L \in \mathbf{MA}$[a,b] if there exists a probabilistic polynomial time verifier V, such that:

1. $\forall x \in L \quad \exists y : \quad |y| = poly(|x|), P(V(x, y) = 1) \geqslant a$
2. $\forall x \notin L \quad \forall y : \quad |y| = poly(|x|), P(V(x, y) = 1) \leqslant b$

Remark 12.

1. The numbers a,$b \in$ [0,1] are such that $a - b \geqslant \text{poly}(|x|^{-1})$
2. One would consider instance x to be the description of a probabilistic circuit taking input y and outputting $V(x,y) \in$ [0,1]

3. **NP** = **MA**[1,0]

Definition 8. A language $L \in \mathbf{QMA}[a,b]$ if there exists a polynomial time quantum verifier V such that:

1. $\forall x \in L \quad \exists\, |\xi\rangle \in [\mathbb{C}^2]^{\otimes \mathrm{poly}(|x|)} : P(V(x, |\xi\rangle) = 1) \geqslant a$
2. $\forall x \notin L \quad \forall\, |\xi\rangle \in [\mathbb{C}^2]^{\otimes \mathrm{poly}(|x|)} \quad P(V(x, |\xi\rangle) = 1) \leqslant b$

Remark 13.

1. The numbers $a,b \in [0,1]$ are such that $a - b \geqslant \mathrm{poly}(|x|^{-1})$
2. One would consider instance x to be the description of a quantum circuit taking input state $|\xi\rangle$ and outputting on the first qubit $V(x,y) \in [0,1]$
3. It is assumed that the verifier has access to a slack register initially in the state $|0\rangle^{\otimes \mathrm{poly}(|x|)}$
4. The quantity $\mathrm{poly}(|x|^{-1})$ is often called, the promise gap and should not be confused with the spectral gap of a Hamiltonian

Chapter 1

The dissertation begins by recalling several established results related to programming the ground states of generalised Ising systems. This presents and builds on my own work as well as the work of others—see the dissertation for citations.

The first chapter begins by considering the relationship between qubit quantum states and Ising penalty functions.

The dissertation begins by defining the quotient ring extension:

$$\mathbb{C}[x_1, x_2, \ldots, x_n] \Big/ x_1, x_2, \ldots, x_n \in \{0,1\} \tag{5}$$

where $x_1, x_2, \ldots, x_n \in \{0,1\}$ the quotient constraint is equivalent to $x_i x_i = x_i$ (idempotence). We arrive at the ring of (qubit) polynomials of type:

$$\{0,1\}^n \to \mathbb{C} \tag{6}$$

by means of the following mapping

$$f(\mathbf{x}) = \sum_{I \in \{0,1\}^n} a_I \mathbf{x}^I \tag{7}$$

where

$$\mathbf{x}^I \stackrel{\text{def}}{=} (x_1)^{i_1}(x_2)^{i_2} \cdots (x_n)^{i_n} \tag{8}$$

and we abuse notation as

$$(x)^0 \stackrel{\text{def}}{=} (1 - x)$$

with $x^1 = x$.

It goes on to state the following propositions.

Proposition 1 (Biamonte (2008))**.** The ring $\mathbb{C}[x_1, x_2, \ldots, x_n] \Big/ \forall i, x_i^2 = x_i$ is graded as

$$\mathbb{C} \oplus \mathbb{C}[x_1] \oplus \cdots \oplus \mathbb{C}[x_n] \oplus \mathbb{C}[x_1, x_2] \oplus \cdots \oplus \mathbb{C}[x_{n-1}, x_n] \oplus \cdots \oplus \mathbb{C}[x_1, x_2, \ldots, x_n] \tag{9}$$

where the quotients are omitted for brevity of notation.

We call an expansion canonical when it is unique up to labeling variables.

Proposition 2. The expansion

$$f(\mathbf{x}) = a_0 + \sum a_i x_i + \sum a_{ij} x_i x_j + \cdots + \sum a_{ij\ldots n} x_i x_j \ldots x_n \tag{10}$$

is canonical.

More generally, the early chapter presents the following:

Lemma 1. The follow isomorphisms hold.

$$\mathbb{C}[x_1, x_2, \ldots, x_n] \Big/ \forall i, x_i^2 = x_i \simeq \mathbb{C}_2^{\otimes n} \simeq \text{diagMat}_{\mathbb{C}}(2^n) \tag{11}$$

By considering the real valued restriction from Proposition 1 and hence Lemma 1, this concept formally connects pseudo Boolean and Ising minimization problems:

Proposition 3 (Operator embedding of Pseudo Boolean forms)**.** Any Pseudo Boolean function

$$f(\mathbf{x}) = \sum_I a_I \mathbf{x}^I \tag{12}$$

gives rise to an operator embedding

$$[f] = \sum_I a_I |I\rangle\langle I| \stackrel{\text{def}}{=} \hat{f} \tag{13}$$

by Lemma 1. The minimisation problems are evidently related as:

$$\min_{x \in \{0,1\}^n} f(x) = x', \tag{14}$$

then

$$\min_{\psi \in \mathcal{A}} \langle \psi | \, \hat{f} \, | \psi \rangle = \langle x' | \, \hat{f} \, | x' \rangle \tag{15}$$

for the appropriate vector space $\mathcal{A}$.

The dissertation then details the practical codomain extension of Karnaugh maps. This is used to derive penalty functions for logical operations. In particular, a deductive method is presented based on Karnaugh maps to derive the following penalty functions. The method to derive these appears novel whereas various penalty functions exist in the literature.

Theorem 1. The following penalty functions embed the logical product $-x_1x_2x_3$ into their lowest energy sector as:

$$-x_1x_2x_3 = \min_{z \in \{0,1\}} z(2 - x_1 - x_2 - x_3), \tag{16}$$

and

$$-x_1x_2x_3 = \min_{z \in \{0,1\}} z(-x_1 + x_2 + x_3) - x_1x_2 - x_1x_3 + x_1. \tag{17}$$

Theorem 2 (Boolean function embedding, Biamonte (2008))**.** Any Boolean function $f(x_1, x_2, \ldots, x_n)$ expressed over the basis $\{\vee, \wedge, \neg\}$ embeds into the spectrum of a Hermitian operator formed by the linear extension of $\{P_0, P_1, \mathbb{1}\}$ by means of

the following maps (18) and (19).

$$\wedge \longrightarrow \otimes \tag{18}$$

$$\vee \longrightarrow + \tag{19}$$

For every (positive polarity, a.k.a. non-negated) Boolean variable x_j we apply

$$x_j \longrightarrow P_1^j. \tag{20}$$

For negated variable $\neg x_j$ we apply

$$\neg x_j \longrightarrow P_0^j. \tag{21}$$

In both cases (20) and (21), $1 \leqslant j \leqslant n$ becomes a spin label index which P^j acts on. Moreover the above mapping induces an operator $\mathcal{H}$ such that

$$\mathcal{H} \left|\mathbf{x}\right\rangle = f(\mathbf{x}) \left|\mathbf{x}\right\rangle \tag{22}$$

for Boolean function $f(\mathbf{x})$ and bit string $\mathbf{x}$.

Theorem 3 (Kernel embedding)**.** A Boolean function $f(x)$ embeds into the kernel of a non-negative Ising penalty function by applying the map from Theorem 2 to the function $g(x, f(x)) = 0$, $g(x, 1 - f(x)) = 1$.

Remark 14. The condition $g(x, 1-f(x)) = 1$ can readily be modified to $g(x, 1-f(x)) \geqslant 1$ leaving the operators constructed by Theorem 2 non-negative with identical kernals.

Definition 9. The set of all two-body Ising Hamiltonians on n spins is defined as: $\Omega_n = \{a_0 + a_1 x_1 + a_2 x_2 + \cdots + a_{12} x_1 x_2 + a_{13} x_1 x_3 + \ldots$

$a_{n-1,n} x_{n-1} x_n | \forall j, k, a_{jk} \in [-l, l] \subset \mathbb{R}\}$.

Remark 15.

Proposition 4. $\nexists H \in \Omega_3 \mid$, $H \geqslant 0$, $\mathrm{Ker}\{H\} = \mathrm{span}\{x, y, z \in \mathbb{B} | z = x \oplus y\}$.

We will also show that the orbits of embedded functions in $\mathrm{Ker}\{H\}$ separate under conjugation of H by σ_x into equivalency classes: $(\mathsf{AND} \sim \mathsf{OR} \sim \mathsf{NAND} \sim \mathsf{NOR}) \in \Omega_3$ and $(\mathsf{XOR} \sim \mathsf{EQV}) \in \Omega_4$.

	bits	probabilistic bits	qubits
state (single unit)	bit $\in \{0,1\}$	real vector $a, b \in \mathbb{R}_+ \qquad a+b=1$ $\vec{p} = a\vec{0}+b\vec{1}$ or $a\,\|0\rangle+b\,\|1\rangle$	complex vector $\alpha, \beta \in \mathbb{C} \;\; \|\alpha\|^2 + \|\beta\|^2 = 1$ $\vec{\psi} = \alpha\vec{0} + \beta\vec{1}$ or $\alpha\,\|0\rangle + \beta\,\|1\rangle$
state (multi-unit)	bitstring $x \in \{0,1\}^n$	prob.distribution (stochastic vector) $\vec{p} = \sum_{x\in\{0,1\}^n} a_x \,\|x\rangle \in [\mathbb{R}^2_+]^{\otimes n}$	wavefunction (complex vector) $\vec{\psi} = \sum_{x\in\{0,1\}^n} \alpha_x \,\|x\rangle \in [\mathbb{C}^2]^{\otimes n}$
operations	Boolean logic	stochastic matrices $\sum_j P_{ij} = 1,\ P_{ij} \geqslant 0$	unitary matrices $U^\dagger U = \mathbf{1}$
component ops	Boolean gates	tensor product of matrices	tensor product of matrices

Table 2 — Summary of deterministic, probabilistic and quantum bits. We use the standard notation that $\mathbb{R}^2_+$ denotes the two-dimensional real vector space with non-negative entries. Likewise, $\mathbb{C}^2$ is the two-dimensional complex vector space. The space of n pbits, n qubits are respectively given by the tensor product of spaces, $[\mathbb{R}^2_+]^{\otimes n}$ and $[\mathbb{C}^2]^{\otimes n}$.

Chapter 2

The second chapter presents a detailed mathematical (structural) comparison between quantum and stochastic mechanics. Table 2 is presented. Then the contents of Table 2 are developed.

Remark 16. Every finite dimensional quantum or stochastic process can be viewed as a (spinless single particle) walk on a graph given by the support of the corresponding time propagator.

For the purpose of comparison, the following definitions are all given in the dissertation.

Remark 17 (Summary of stochastic versus quantum walks)**.** G is a simple graph. Labeling the nodes of G lifts to specify:

1. A the adjacency matrix (generator of a quantum walk).
2. D the diagonal matrix of the degrees.
3. $\mathcal{L}$ the symmetric Laplacian (generator of stochastic and quantum walks), which when normalized by D returns both:

	quantum mechanics	**stochastic mechanics**
state	vector $\psi \in \mathbb{C}^n$ with $$\sum_i \lvert\psi_i\rvert^2 = 1$$	vector $\psi \in \mathbb{R}^n$ with $$\sum_i \psi_i = 1$$ and we typically insist that, $$\psi_i \geq 0$$
observable	$n \times n$ matrix $\mathcal{O}$ with $$\mathcal{O}^\dagger = \mathcal{O}$$ where $(\mathcal{O}^\dagger)_{ij} \stackrel{\text{def}}{=} \overline{\mathcal{O}}_{ji}$	vector $\mathcal{O} \in \mathbb{R}^n$
expected value	$\langle\psi\lvert\mathcal{O}\rvert\psi\rangle \stackrel{\text{def}}{=} \sum_{i,j} \overline{\psi}_i \mathcal{O}_{ij} \psi_j$	$\langle\mathcal{O}\psi\rangle \stackrel{\text{def}}{=} \sum_i \mathcal{O}_i \psi_i$
symmetry (linear map sending states to states)	unitary $n \times n$ matrix: $$UU^\dagger = U^\dagger U = \mathbb{1}$$	stochastic $n \times n$ matrix: $$\sum_i U_{ij} = 1, \quad U_{ij} \geq 0$$
symmetry generator	self-adjoint $n \times n$ matrix: $$\mathcal{H} = \mathcal{H}^\dagger$$	infinitesimal stochastic $n \times n$ matrix: $$\sum_i \mathcal{H}_{ij} = 0, \quad i \neq j$$ $$\Rightarrow \ \mathcal{H}_{ij} \leq 0$$
symmetries from symmetry generators	$U(t) = \exp(-\imath t\mathcal{H})$	$U(t) = \exp(-t\mathcal{H})$
equation of motion	$$\imath\frac{d}{dt}\psi(t) = \mathcal{H}\psi(t)$$ with solution $\psi(t) = \exp(-\imath t\mathcal{H})\psi(0)$	$$\frac{d}{dt}\psi(t) = -\mathcal{H}\psi(t)$$ with solution $\psi(t) = \exp(-t\mathcal{H})\psi(0)$

Table 3 — Summary of quantum versus statistical mechanics.

3.1 S the generator of the uniform escape stochastic walk and

3.2 Q the quantum walk generator to which $\mathcal{L}$ is similar.

Several results are derived, leading to the subadditivity of entropy of stochastic generators:

Remark 18. A simple undirected graph with edges weighted by real numbers gives rise to a *generalized symmetric adjacency matrix*. For edges labeled l and m weighted by $w \in \mathbb{R}$, the l-m^{th} entry of the corresponding adjacency matrix is w.

Definition 10. A *generalized Laplacian* arises as

$$\mathcal{L} = \mathcal{D} - \mathcal{A} \tag{23}$$

where A is a generalized symmetric adjacency matrix and D stores on its diagonal entries the sums of the corresponding rows of A.

Theorem 4 (Biamonte-DeDomenico 2016)**.** Given two generalized Laplacians and their sum $\mathcal{L}_C = \mathcal{L}_A + \mathcal{L}_B$, and corresponding Gibbs state density matrices $\rho_{\mathcal{C}} = e^{\beta(\mathcal{L}_{\mathcal{A}}+\mathcal{L}_{\mathcal{B}})}/\mathcal{Z}$, the von Neumann entropy $S(\rho) = Tr\{\rho \ln_2 \rho\}$ is subadditive as,

$$S(\rho_{\mathbf{C}}) \leqslant S(\rho_{\mathbf{A}}) + S(\rho_{\mathbf{B}}). \tag{24}$$

Remark 19. We adopt the notation that $S(\rho_A) \equiv S_A$, $S(\rho_B) \equiv S_B$, etc.

The second chapter concludes by presenting several methods to find minimal graph properties on a quantum processor.

Chapter 3

Techniques from the theory of tensor networks can apply to quantum circuits. In chapter 3 the following theorem on generating families of tensor networks is proven.

Theorem 5 (Minimal Stabilizer Tensor Generators)**.** The following generating tensors are sufficient to simulate any stabilizer quantum circuit:

(a) a vector $|t\rangle \stackrel{\text{def}}{=} |0\rangle + \imath\,|1\rangle$,
(b) the Hadamard gate and
(c) the XOR- and COPY tensors and
(d) a covector $\langle +| \stackrel{\text{def}}{=} \langle 0| + \langle 1|$.

Remark 20. The Gottesman–Knill theorem states that stabilizer circuits—circuits that only consist of gates from the normalizer of the qubit Pauli group, a.k.a. Clifford group—can be simulated in polynomial time on a probabilistic classical computer.

The dissertation constructs a sequence of graphical rewrites to establish this theorem by algebraic properties of tensor contraction, namely:

Theorem 6 (Graphical Proof of the Gottesman–Knill Theorem)**.** For n-qubits acted on by L Clifford gates, there exists a confluent sequence of rewrites, that establishes the Gottesman–Knill theorem in $\mathcal{O}(\text{poly}(n, L))$ steps.

Chapter 4

We then consider the minimisation of Hamiltonians by parameterised quantum circuits. This provides an illustrative connection between computational and physical complexity, stated and defined in the early chapter step wise. The variational model contains the following ingredients which will be further defined:

1. **States**. A vector of real parameters $\boldsymbol{\theta}$ sets a circuit to produce $|\psi(\boldsymbol{\theta})\rangle$.
2. **Measurements**. Expected values of a Pauli strings, $\bigotimes_{j=1}^{n} \sigma_j^{\alpha_j}$ for $\alpha_j \in \{0,1,2,3\}$ can be computed for each $|\psi(\boldsymbol{\theta})\rangle$.
3. **Compute cost function**. A cost function defined by a weighted sum of expected values is computed for each $|\psi(\boldsymbol{\theta})\rangle$.
4. **Outer-loop optimization**. Classical optimization routines update parameters $\boldsymbol{\theta} \to \boldsymbol{\theta}_\star$.

Definition 11 (Variational Statespace—Biamonte (2021))**.** The variational statespace of a p-parameterized n-qubit state preparation process is the union

of $|\psi(\boldsymbol{\theta})\rangle$ over all possible assignments of real numbers $\boldsymbol{\theta}$:

$$\Gamma = \bigcup_{\boldsymbol{\theta}\in(0,2\pi]^{\times p}} |\psi(\boldsymbol{\theta})\rangle\,. \tag{25}$$

Definition 12 (Variational Sequence)**.** A variational sequence specifies parameters to prepare a state in a variational statespace. It can be given by defining a specific sequence of gates or by specifying control parameter values.

Definition 13 (Variational principle)**.** A *variational principle* is a problem specific reduction to that of finding extrema of an objective function. Variational quantum computation considers the normalized minimization:

$$\min_{|\psi(\boldsymbol{\theta})\rangle\in\Gamma\subset V_n} \langle\psi(\boldsymbol{\theta})|\, H\, |\psi(\boldsymbol{\theta})\rangle \geqslant \min_{|\psi\rangle\in V_n} \langle\psi|\, H\, |\psi\rangle\,. \tag{26}$$

Remark 21. Alternative NISQ approaches might minimise the variance

$$\min(\langle\mathcal{H}^2\rangle - \langle\mathcal{H}\rangle^2) \geqslant 0 \tag{27}$$

which vanishes if and only if $|\psi\rangle$ is an eigenstate of $\mathcal{H}$.

Cost function implementation proceeds by applying the fact that an expected value of a sum is a sum of expected values.

$$\langle\psi|\,\mathcal{H}\,|\psi\rangle = \langle\psi|\sum_k h_k \bigotimes_{j=1}^{n} \sigma_j^{\alpha_j(k)}\,|\psi\rangle = \sum_k h_k\,\langle\psi|\bigotimes_{j=1}^{n}\sigma_j^{\alpha_j(k)}\,|\psi\rangle \tag{28}$$

where h_k is a real number and $\bigotimes_{j=1}^{n}\sigma_j^{\alpha_j(k)}$ is a Pauli string for $\alpha_j \in \{0,1,2,3\}$.

Remark 22 (Iteration)**.** Given copies of $|\psi\rangle$, measuring $\bigotimes_{j=1}^{n}\sigma_j^{\alpha_j(k)}$ repeatedly gives an estimate for each $\langle\psi|\bigotimes_{j=1}^{n}\sigma_j^{\alpha_j(k)}\,|\psi\rangle$ separately.

Remark 23. Whereas the objective function can be evaluated term-wise, achieving tolerance $\sim\varepsilon$ requires $\sim\varepsilon^{-2}$ measurements—see Hoeffding's inequality.

Definition 14 (Objective Function Cardinality)**.** The number of terms in the Pauli basis $\{\mathbb{1}, X, Y, Z\}^{\otimes n}$ needed to express an objective function.

Example 1. Let $\mathcal{H} = \sum_k h_k \bigotimes_{j=1}^{n}\sigma_j^{\alpha_j(k)}$ for coefficients h_k and Pauli strings $\bigotimes_{j=1}^{n}\sigma_j^{\alpha_j(k)}$. Then $|\mathcal{H}|_{\text{card}} = \sum_k (h_k)^0$.

Definition 15 (Bounded Objective Function—Biamonte (2021))**.** A family of objective functions is *efficiently computable* when uniformly generated by calculating the expected value of an operator with poly(n) bounded cardinality over

$$\Omega \subset \{\mathbb{1}, X, Y, Z\}^{\otimes n}. \tag{29}$$

Definition 16 (Poly-Computable Objective Function—Biamonte (2021))**.** An objective function

$$f\colon \left|\phi\right\rangle^{\times \mathcal{O}(\mathrm{poly}(n))} \to \mathbb{R}_+ \tag{30}$$

is called poly-computable provided poly(n) independent physical copies of $|\phi\rangle$ can be efficiently prepared to evaluate a bounded objective function.

Definition 17 (Accepting a Quantum State—Biamonte (2021))**.** An objective function f *accepts* $|\phi\rangle$ when given $\mathcal{O}(\mathrm{poly}\ n)$ copies of $|\phi\rangle$,

$$f(\left|\phi\right\rangle^{\times \mathcal{O}(\mathrm{poly}(n))}) = f(\left|\phi\right\rangle, \left|\phi\right\rangle, \cdots, \left|\phi\right\rangle) < \Delta \tag{31}$$

evaluates strictly less than a chosen real parameter $\Delta > 0$.

Theorem 7 (Energy to Overlap Theorem—Biamonte (2021))**.** Let non-negative $\mathcal{H} = \mathcal{H}^\dagger \in \mathscr{L}(\mathbb{C}_d)$ have spectral gap Δ and non-degenerate ground eigenvector $|\psi\rangle$ of eigenvalue 0. Consider then a unit vector $|\phi\rangle \in \mathbb{C}_d$ such that

$$\left\langle\phi\right| \mathcal{H} \left|\phi\right\rangle < \Delta \tag{32}$$

it follows that

$$1 - \frac{\left\langle\phi\right| \mathcal{H} \left|\phi\right\rangle}{\Delta} \leqslant |\left\langle\phi|\psi\right\rangle|^2 \leqslant 1 - \frac{\left\langle\phi\right| \mathcal{H} \left|\phi\right\rangle}{\mathrm{Tr}\{\mathcal{H}\}}. \tag{33}$$

Several constructions related to quantum approximate optimization using short parameterised quantum circuits are subsequently developed. A general bound applicable to short circuits is then given.

Consider a pure n-qubit state $|\psi\rangle$.

Definition 18. Bipartite Rank is the Schmidt number (the number of non-zero singular values) across any reduced bipartite density state from $|\psi\rangle$ (i.e. $\lceil n/2 \rceil$ qubits).

Definition 19. An ebit is a unit of entanglement contained in a maximally entangled two-qubit (Bell) state.

Remark 24. A quantum state with q ebits of entanglement (quantified by any entanglement measure) contains the same amount of entanglement (in that measure) as q Bell states.

If a task requires r ebits, it can be done with r or more Bell states, but not with fewer. Maximally entangled states in $\mathbb{C}^d \otimes \mathbb{C}^d$ have $\log_2(d)$ ebits of entanglement.

The dissertation then presents and proves the following:

Theorem 8 (Combinatorial quantum circuit area law—Biamonte-Morales-Koh (2020))**.** Let c be the depth of 2-qubit controlled NOT gates in an ansatz circuit. Then the maximum possible number of ebits is $\min\{\lfloor n/2 \rfloor, c\}$.

Finally, the chapter presents the definition of an effect the dissertation author discovered and published with coauthors.

Definition 20. Let $|\psi\rangle$, be the ansatz states generated from a p–depth QAOA circuit. Then

$$f = \min_{\psi \subset \mathcal{H}} \langle\psi| \mathcal{V} |\psi\rangle - \min_{\phi \in \mathcal{H}} \langle\phi| \mathcal{V} |\phi\rangle , \tag{34}$$

characterises the limiting performance of QAOA.

The R.H.S. of equation (34) can be expressed as a function, $f(p,\alpha,n)$.

Proposition 5 (Reachability Deficit—with Akshay et al. 2020)**.** For $p \in \mathbb{N}$ and fixed problem size, $\exists\ \alpha > \alpha_c$ such that f from (34) is non-vanishing. This is a reachability deficit.

Chapter 5

Chapter 5 develops a universal model of variational quantum computation. The early chapter related to programming diagonal Hamiltonin ground states. Chapter's 5 and 6 focus on the non-diagonal case.

The dissertation then goes on to construct Hermitian $\mathcal{H} \in \mathcal{L}(\mathbb{C}_2^{\otimes n})$ with $\mathcal{H} \geqslant 0$ and non-degenerate $|\psi\rangle \in \mathbb{C}_2^{\otimes n}$ as $\mathcal{H}|\psi\rangle = 0$. Define

$$P_\phi = \sum_{i=1}^{n} |1\rangle\langle 1|^{(i)} = \frac{n}{2}\left(\mathbb{1} - \frac{1}{n}\sum_{i=1}^{n} Z^{(i)}\right) \tag{35}$$

and consider (35) as the initial Hamiltonian, preparing state $|0\rangle^{\otimes n}$.

We will act on (35) with a sequence of gates $\prod_{l=1}^{L} U_l$ corresponding to the circuit being simulated as

$$h(k) = \left(\prod_{l=1}^{k\leqslant L} U_l\right) P_\phi \left(\prod_{l=1}^{k\leqslant L} U_l\right)^\dagger \geqslant 0 \tag{36}$$

which isospectral on (35).

Lemma 2 (Clifford Gate Cardinality Invariance)**.** For C a Clifford gate and $h \in \mathrm{span}_{\mathbb{R}}\{\bigotimes_{l=1}^{n} \sigma_l^{\alpha_l} \mid \alpha_l = 0,1,2,3\}$, $|h|_{\mathrm{card}} = |ChC^\dagger|_{\mathrm{card}}$.

Remark 25. The algebraic k-locality of (36) is not invariant under Clifford conjugation.

Remark 26. Non-Clifford gates increase the cardinality of (36) by exponentially and so must be logarithmically bounded from above, restricting to p gate circuit's with $\mathcal{O}(\mathrm{poly}\ln p)$ non-Clifford single qubit gates.

We will then consider embedding general quantum circuits into Hamiltonian ground states.

Two notions of universality are common in the literature:

1. Strongly universal means a system is fully controllable and able to approximate any state.
2. Computationally universal means that any quantum circuit can be efficiently simulated by this model.

Remark 27 (with Morales and Zimboras QIP **19**:291 (2020))**.** One can simulate general p-depth circuits containing two-qubit gates with ansatze circuits of $\mathcal{O}(\mathrm{poly}(p))$ depth.

Theorem 9 (Biamonte PRA 103:L030401 (2021))**.** Let $\Pi_{l=1}^{L} U_l |0^n\rangle$ be an L-gate quantum circuit preparing state $|\psi\rangle$ on n-qubits and containing $L-c$ non-Clifford

gates. Then there exists a non-negative Hamiltonian $\mathcal{H}$ on n-qubits with $|\mathcal{H}|_{\text{card}} = \mathcal{O}\left(\text{poly}(c, e^{L-c})\right)$, gap Δ and $\ker\{\mathcal{H}\} = \text{span}\{\Pi_{l=1}^{L} U_l |0^n\rangle\}$. In particular, if $|\phi\rangle$ is such that

$$0 \leqslant \langle\phi| \mathcal{H} |\phi\rangle < \Delta \tag{37}$$

then it follows that

$$1 - \frac{\langle\phi| \mathcal{H} |\phi\rangle}{\Delta} \leqslant |\langle\phi|\psi\rangle|^2 \leqslant 1 - \frac{\langle\phi| \mathcal{H} |\phi\rangle}{\text{Tr}\{\mathcal{H}\}}. \tag{38}$$

For some U a Clifford gate, Lemma 2 shows that the cardinality is invariant. Non-Clifford gates increase the cardinality by factors $\mathcal{O}(e^{L-c})$ and so must be logarithmically bounded from above. Hence, telescopes bound the number of expected values by restricting to circuit's with

$$k \sim \mathcal{O}(\text{poly} \ln n)$$

general single qubit gates. Clifford gates do however modify the locality of terms appearing in the expected values.

Chapter 5 then presents then proves the following theorem (10) which establishes universality of the variational model of quantum computation.

Theorem 10 (Universal Objective Function—Biamonte (2021))**.** Consider a quantum circuit of L gates on n-qubits producing state $\prod_l U_l |0\rangle^{\otimes n}$. Then there exists an objective function (Hamiltonian, $\mathcal{H}$) with non-degenerate ground state, cardinality $\mathcal{O}(L^2)$ and spectral gap $\Delta \geqslant \mathcal{O}(L^{-2})$ acting on $n + \mathcal{O}(\ln L)$ qubits such that acceptance implies efficient preparation of the state $\prod_l U_l |0\rangle^{\otimes n}$. Moreover, a variational sequence exists causing the objective function to accept.

The proof follows from several lemma. Degeneracy is first lifted. We let $P_0 = |0\rangle\langle 0|$.

Lemma 3 (Degeneracy Lifting)**.** A tensor product of a projector on the first clock qubit with a telescope

$$\mathcal{H}_{\text{in}} = V \left(\sum_{i=1}^{n} P_1^{(i)} \right) V^\dagger \otimes P_0 \tag{39}$$

lifts the degeneracy of $\mathcal{H}_{\text{prop}}$ and the history state with fixed input as

$$\frac{1}{\sqrt{L+1}} \sum_{t=0}^{L} \prod_{l=1}^{t} U_l (V |0\rangle^{\otimes n}) \otimes |t\rangle \tag{40}$$

becomes the non-degenerate ground state of $J \cdot \mathcal{H}_{\text{in}} + K \cdot \mathcal{H}_{\text{prop}}$ for real $J, K > 0$.

The penalty function is gaped and omits a log-space embedding.

Lemma 4 (Gap Existence)**.** For appropriate non-negative J and K, the operator $J \cdot \mathcal{H}_{\text{in}} + K \cdot \mathcal{H}_{\text{prop}}$ is gapped.

Note that in the theory of adiabatic quantum computation, several authors bound the gap of operators such as $J \cdot \mathcal{H}_{\text{in}} + K \cdot \mathcal{H}_{\text{prop}}$. One such lower bound is L^{-3} for an L gate circuit [SIAM Journal of Computing 37(1):166 (2007)].

Lemma 5 (Logspace Embedding $\mathcal{H}_{\text{prop}}$)**.** The clock space of $\mathcal{H}_{\text{prop}}$ embeds into $\mathcal{O}(\ln L)$ slack qubits, leaving the ground space of $J \cdot \mathcal{H}_{\text{in}} + K \cdot \mathcal{H}_{\text{prop}}$ and the gap invariant.

The dissertation then proves acceptance and derives the bound, noting that one must add M identity gates to boost the probability of the desired circuit output state $|\phi\rangle = \Pi_{l=1}^{L} U_l |0\rangle^{\otimes n}$. The telescoping construction, we have that

$$1 - \frac{\langle \phi | \mathcal{H} | \phi \rangle}{L^{-3}} \leqslant |\langle \phi | \psi_{\text{hist}} \rangle|^2 = \frac{1}{1 + \frac{L+1}{M}} \tag{41}$$

whenever $\langle \phi | \mathcal{H} | \phi \rangle < L^{-3}$. For large enough $M > L$, the right hand side of (41) approaches unity, implying acceptance.

Chapter 6

Remark 28. Kitaev et al. established that sparse Hamiltonian's restricted to have at most 5-body bounded strength interactions have a ground state energy problem which is complete for the quantum analog of the complexity class **NP** (QMA-hard).

Definition 21. The k-local Hamiltonian problem: The input is a k-local Hamiltonian acting on n qubits, which is the sum of poly many Hermitian matrices that act on only k qubits. The input also contains two numbers $a < b \in [0,1]$, such that $\frac{1}{b-a} = \mathcal{O}(n^{-c})$ for some constant c. The problem is to determine whether the smallest eigenvalue of this Hamiltonian is less than a or greater than b, promised that one of these is the case.

Remark 29. The k-local Hamiltonian admits an energy decision problems with is QMA-complete for $k \geqslant 2$. The minimisation of k-local Hamiltonians is QMA-hard for $k \geqslant 2$. We seek to determine the simplest 2-local QMA-hard Hamiltonian to embed computational problems into a Hamiltonian for practical means.

The dissertation then develops and proves the following theorems.

Remark 30 (Real Hamiltonians)**.** We call Hamiltonian's expressed in the real subset of the Pauli basis, *real Hamiltonians*. That is, qubit Hamiltonians that contain no tensor product terms with odd numbers of Y operator(s). The corresponding ground state energy problem is called Real Hamiltonian.

Lemma 6. The ground state energy decision problem Real Hamiltonian is QMA-hard.

Remark 31 (Complexity (Sketch))**.** Given a Hamiltonian on n qubits, determine if $\min_{|\psi\rangle \in V_n} \langle\psi| H |\psi\rangle$ is below b or above a for $a, b \in [0,1]$ and $b - a \geqslant \text{poly}(n^{-1})$.

Remark 32 (Universality (Sketch))**.** A computationally universal set of real valued gates is embedded to act in ground states of (42) and (43).

Theorem 11 (Biamonte-Love (2008))**.** The ground energy decision problem *ZZXX Hamiltonian* is QMA-hard, given as:

$$H_{\text{ZZXX}} = \sum_i h_i Z_i + \sum_{i,j} J_{ij} Z_i Z_j + \sum_{i,j} K_{ij} X_i X_j. \tag{42}$$

Theorem 12 (Biamonte-Love (2008))**.** The ground energy decision problem *ZX Hamiltonian* is QMA-hard, given as:

$$H_{\text{ZX}} = \sum_i h_i Z_i + \sum_{i,j} J_{ij} Z_i X_j. \tag{43}$$

The Hamiltonian (44) (that is, 45) can create effective $Y \otimes Y$ (that is, $Z \otimes Z \otimes Z$) interactions with error ε using one slack bit acted on by a term $\sim \varepsilon^{-4} Z$ (that is, $\sim \varepsilon^{-5} X$).

Theorem 13 (with Cao-et al. (2015))**.** The Hamiltonian

$$H_{\mathrm{ZZXX}} = \sum_i h_i Z_i + \sum_i \Delta_i X_i + \sum_{i,j} J_{ij} Z_i Z_j + \sum_{i,j} K_{ij} X_i X_j. \tag{44}$$

emulates a $Y \otimes Y$ interaction with $\delta = \mathcal{O}(\varepsilon^{-4})$ given one slack qubit.

Theorem 14 (with Cao-et al. (2015))**.** The Hamiltonian

$$H_{\mathrm{Ising,X}} = \sum_i h_i Z_i + \sum_i \Delta_i X_i + \sum_{i,j} J_{ij} Z_i Z_j. \tag{45}$$

emulates the $Z \otimes Z \otimes Z$ interaction with $\delta = \mathcal{O}(\varepsilon^{-5})$ given one slack qubit.

Conclusion

The conclusion presents and discusses the implications of efficiently checkable quantum versus classical minimization problems. It also presents some future research directions.

Anticipated computational resources to determine ground state energy and calculate energy relative to a state have been conjectured. In Table 4 I have summarized what is known/conjectured regarding efficiently checkable minimisation problems. Therein 'Restricted Ising' denotes problems known to be in P. (*) denotes conjectures. Electronic structure problem instances have constant maximum size so are assumed to be in BQP whereas the ZZXX model is QMA-hard.

Table 4 — Hamiltonian complexity micro zoo

Problem Hamiltonian	**Finding Ground Energy** (Classical / Quantum)	**Calculating State Energy** (Classical / Quantum)
1-Local Hamiltonian	Polynomial	Polynomial
2-Local Ising	Exp	Polynomial
Electronic Structure	*Exp	*Exp / Polynomial
ZZXX Model	Exp	*Exp / *Polynomial

TWENTY PRIMARY RESEARCH ARTICLES CONSTITUTING THE DISSERTATION CONTENTS

1. Akshay V. et al. Reachability Deficits in Quantum Approximate Optimization // Phys. Rev. Lett. 2020. Vol. 124, № 9. P. 090504.
2. Biamonte J.D., Morales M.E.S., Koh D.E. Entanglement scaling in quantum advantage benchmarks // Phys. Rev. A. 2020. Vol. 101, № 1. P. 012349.
3. Whitfield J.D., Faccin M., Biamonte J.D. Ground State Spin Logic // EPL (Europhysics Letters). 2012. Vol. 99, № 5. P. 57004.
4. Biamonte J.D., Love P.J. Realizable Hamiltonians for universal adiabatic quantum computers // Phys. Rev. A. 2008. Vol. 78, № 1. P. 012352.
5. Whitfield J.D., Biamonte J., Aspuru-Guzik A. Simulation of electronic structure Hamiltonians using quantum computers // Molecular Physics. 2011. Vol. 109, № 5. P. 735–750.
6. Biamonte J.D. et al. Adiabatic quantum simulators // AIP Advances. 2011. Vol. 1, № 2. P. 022126.
7. Biamonte J.D., Morton J., Turner J. Tensor Network Contractions for #SAT // Journal of Statistical Physics. 2015. Vol. 160, № 5. P. 1389–1404.
8. Cao Y. et al. Hamiltonian gadgets with reduced resource requirements // Physical Review A. 2015. Vol. 91, № 1.
9. Faccin M. et al. Community Detection in Quantum Complex Networks // Phys. Rev. X. 2014. Vol. 4, № 4. P. 041012.
10. Faccin M. et al. Degree Distribution in Quantum Walks on Complex Networks // Phys. Rev. X. 2013. Vol. 3, № 4. P. 041007.

11. Morton J., Biamonte J. Undecidability in tensor network states // Phys. Rev. A. 2012. Vol. 86, № 3. P. 030301.
12. Denny S.J. et al. Algebraically contractible topological tensor network states // J. Phys. A: Math. Theor. 2012. Vol. 45, № 1. P. 015309.
13. Morales M.E.S., Tlyachev T., Biamonte J. Variational learning of Grover's quantum search algorithm // Physical Review A. 2018. Vol. 98, № 6.
14. Biamonte J. Charged string tensor networks // Proceedings of the National Academy of Sciences. 2017. Vol. 114, № 10. P. 2447–2449.
15. De Domenico M., Biamonte J. Spectral Entropies as Information-Theoretic Tools for Complex Network Comparison // Phys. Rev. X. 2016. Vol. 6, № 4. P. 041062.
16. Biamonte J. Universal Variational Quantum Computation // Phys. Rev. A. 2021. Vol. 103, № 3. P. 030401.
17. Kardashin A., Uvarov A., Yudin D., Biamonte J. Certified variational quantum algorithms for eigenstate preparation // Phys. Rev. A. 2020. Vol. 102, № 5. P. 052610.
18. Morales M.E.S., Zimbor Z., Biamonte J. On the universality of the quantum approximate optimization algorithm // Quantum Information Processing. 2020. Vol. 19, № 9., P. 291.
19. Uvarov A., Kardashin, A, Biamonte J. Machine learning phase transitions with a quantum processor // Physical Review A. 2020. Vol. 102, № 7. P.012415.
20. Baez J., Biamonte J.D. Quantum Techniques in Stochastic Mechanics. World Scientific Publishing Co Pte Ltd, 2018.