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ON THE THEORY OF MODERN QUANTUM ALGORITHMS

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EXTENDED THESIS ABSTRACT

Technical summary

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).[1] Unlike traditional textbook quantum algorithms, quantum algorithms executed on NISQ devices operate in the presence of systematic and random errors. 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 quantum assisted a.k.a. quantum accelerated annealing. While not a general purpose quantum computer in their current form (though universality is possible with further developments [2]), quantum annealers—such as those from D-Wave—have been readily available for several years. Annealers are already in wide use for research and prototyping purposes. While the capabilities of modern day annealers are fairly well understood, their universal counterparts are not.

Understanding the scope of applications of NISQ-era devices—such as when and how we might expect a quantum speedup and exactly how to program these new machines—is a subject of rapid development. As the title implies, *Modern Quantum Algorithms*, entails precisely the scope of this thesis. Ideas from Hamiltonian complexity and the theory of ground states of physical and synthetic (emulated) Hamiltonians act as a sort of golden thread, uniting variational computation with a better established theory of ground state computation. This thesis approaches quantum programming at this intersection with the idea that it should be readable to graduate students.

While a vast number of open questions still remain, on the optimistic side, Google has recently demonstrated quantum computational supremacy [3]. This however is an adversarial game biased to give the quantum processors an evident advantage. Indeed, the task itself is not practical. Simply put, it represents an

[1]Noisy Intermediate-Scale Quantum (NISQ) [1].

elegant abstraction to illustrate that classical computers suffer when emulating quantum systems, even if the quantum computer is error prone. While interesting as a milestone, it is not clear how close this result [3] has placed more useful applications. The questions one might ask are numerous and painfully under explored. Studying some of these questions motivates this thesis: we develop some of the tools to do so. We also conclude with a survey of open problems in § 7.

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. These questions are of such significance today that recent dedicated programs have been initiated around the globe devoted to their solution (we've written on this global quest with coauthors here [4; 5]). This thesis sketches a pathway towards these contemporary challenges, providing insights and partial solutions to several areas of growing interest. Readers are assumed to be familiar with quantum computation at the level of one of the common text books, e.g. [6].

The goal(s) of this dissertation

We aim to present a consistent and general unified framework, which conceptually binds together many of the tools used across contemporary quantum programming. The unifying focus is on properties of ground states of Hamiltonians:

(i) Programming ground states is required in adiabatic quantum computation and other models of ground state annealing.

(ii) It is also central to physics and chemistry simulation algorithms that are anticipated to be promising future applications on quantum computers.

(iii) Finally, the variational model of quantum computation is stated by means of a ground state energy optimisation problem that utilises a classical to quantum feedback loop.

The goal is then simply stated. We present a coherent view that 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; and (iii) the variational approach to Hamiltonian minimisation. In doing so, our pedagogical presentation should be accessible to readers familiar with a standard text books on the subject, such as [6].

Tasks performed to achieve dissertation goals

To present the most central portions of the theory underpinning the contemporary quantum algorithms applications drive, we have to focus on Hamiltonian ground states as they arise in practical applications of quantum enhanced algorithms. To accomplish that goal, care was taken to introduce the concepts in a pedagogical order. The logical starting point is understanding how to program ground states of Ising models.

The thesis begins by recalling several established results related to programming the ground states of generalised Ising systems. This presents and builds on my own work [7; 8], as well as the work of others—see the review [9]. The topic naturally extends towards more recent work done in collaboration on the area of the *computational phase transition signature* of 3-SAT [10]. This provides an illustrative connection between computational and physical complexity, stated and defined in the early chapter step wise. Therefore, to build the first element of the thesis we must present a comprehensive summary of the results on ground state embeddings as they apply to the Ising model. In the early chapter, we don't consider time evolution: we consider static Hamiltonians and Gibbs states.

We next must explain the quantum algorithm called, phase estimation. We survey phase estimation by comparing the evolution of quantum versus stochastic systems. This adds time dependence and extends the elements we established in the early chapter. We then must connect this to the quantum circuit model. From this vantage point, we then introduce the contemporary variational algorithms (QAOA in particular).

With these elements established, the thesis then presents the unviersal model of variational quantum computation. In doing so, the early chapters ideas related to programming diagonal Hamiltonin ground states must be revisited and revised to apply to the non-diagonal case. After doing that, the final chapter also recalls the more general approach to shape Hamiltonian ground states, based on gadget perturbation theory.

Main statements defended

The early chapter establishes several elementary results.

1. Logic operations (gates) can be faithfully embedded into the low-energy sector of Ising spins [7; 8]. (including several further implications)
2. The computational phase transition has a signature in Gibbs sampling [4] and is thus (in principle) detectable with near-term physics based processors.

The first of these assertions is based on (and defended through) deductive reasoning [7; 8] while the second is empirically established [10].

Next, the thesis establishes several relationships between stochastic and quantum walks on graphs. These results were published as parts of several collaborations (see the review [11]) and are briefly summarized herein.

The graphical tensor calculus, called the ZX calculus sometimes, is used to recover the Gottesman–Knill theorem (see [12]). In other words, § 3 establishes that:

3. Example: The ZX tensor rewrite system admits a poly-time terminating rewrite sequence establishing the Gottesman–Knill theorem. To establish this we also prove Theorem 11. We then state Theorem 12.

This follows by deduction, thereby formally defending the assertion (3). Such results are included largely to illustrate and introduce background materials on tensor networks and quantum circuits.

The thesis continues by relating Grover search and variational algorithms [13]. The thesis develops and partially extends a quantum gate factorization method originating in [14]. Finally, the thesis presents the combinatorial quantum circuit area law [15],

4. The combinatorial quantum circuit area law bounds the ebits across any bipartion of qubits acted on by a quantum circuit comprised of local unitaries and CNOT gates. More formally,

   (Lemma 12—[15; 16]) Let c be the depth of 2-qubit CNOT gates in the n-qubit hardware-efficient ansatz. Then the maximum possible number of ebits across any bipartition is $E_b = \min\{\lfloor n/2 \rfloor, c\}$.

The result (4, Lemma 12) is established deductively. The chapter then concludes showing that:

5. An order parameter exists that quantifies problem structure in variational algorithms. The order parameter correlates with ansatz depth (meaning there exist problem instances that require high depth ansatz circuits). We call this a "reachability deficit."

This result (5), as recently published in [17] is established through a combination of deduction and empirical evidence (5).

We follow the statement (5) with a proof related to the variational model [16], namely:

6. The variational model formalizes the iterative classical-to-quantum feedback loop to create a universal model of quantum computation stated in terms of objective function minimization [16]. More formally, we establish two primary results.

   (Lemma 14) Consider $\prod_l U_l |0\rangle^{\otimes n}$ a L-gate quantum circuit preparing state $|\psi\rangle$ on n-qubits and containing not more than $\mathcal{O}(\text{poly} \ln n)$ non-Clifford gates. Then there exists a Hamiltonian $\mathcal{H} \geqslant 0$ on n-qubits with poly(L, n) cardinality, a (L, n)-independent gap Δ and non-degenerate ground eigenvector $\propto \prod_l U_l |0\rangle^{\otimes n}$. In particular, a variational sequence exists causing the Hamiltonian to accept $|\phi\rangle$ viz., $0 \leqslant \langle\phi| \mathcal{H} |\phi\rangle < \Delta$ then Theorem 13 implies stability (Theorem 13).

(Theorem 14) 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 that the variational model of quantum computation is universal [16] is defended formally by deductive reasoning. The proof involves introducing constructions that differ from known results. The proof strategy goes as follows.

6.1 Stability theorem (relates expected energy with state-overlap)—Theorem 13.

6.2 Telescopes (the backbone construction)—Lemma 14

6.2.1 Clifford invariance of penalty functions—Lemma 15

6.2.2 Existence of an accepting sequence

6.3 Modify Feynman-Kitaev construction

6.3.1 Set input with a telescope

6.3.2 Prove existence of a gap—Lemma 17

6.3.3 Prove log qubit clock embedding—Lemma 18

6.3.4 Prove boosting lemma → show existence of an accepting sequence (given by the quantum circuit being emulated)—Lemma 19

The result (6) assumes a noise free system. Furthermore, the optimization problem typically encountered in variational quantum computation is avoided as follows. Though somehow artificial, the circuit being emulated itself provides the control sequence which causes the corresponding objective function to accept.

Finally, the thesis concludes with an overview of the perturbation theory technique used to interelate Hamiltonian models by showing how to emulate new- and higher order interactions using present Hamiltonian terms [18; 19]. Namely, § 6 contains a proof that:

7. The two-body model Hamiltonian

$$\mathcal{H} = \sum_{i<j} J_{ij} Z_i Z_j + \sum_{i<j} K_{ij} X_i X_j$$

is (i) computationally universal for adiabatic quantum computation and (ii) admits a **QMA**-complete ground state energy decision problem [7].

The conclusion (§ 7) surveys some contemporary open problems.

Scientific novelty

The primary results defended in this thesis have appeared in peer reviewed journals. I hope the thesis itself culminates to produce an emergent type of novelty for its readers! Indeed, the thesis has an over arching theme: modern quantum programming is presented in terms of computational properties of ground states. These concepts have played a central role in my own research. The broadness of scope to have these concepts presented together with a unifying purpose has certainly not something I've seen done before. While the more established results presented in this thesis are easily identified, perhaps the most novel recent result is the proof that the variational model is computationally universal. It combines a number of known results, tailors them to specific ends and introduces several new lemmas and theorems to support the development and establishment of the theorem(s).

Practical significance

Variational methods represent an attractive near-term approach due to the ease at which these algorithms can be realized experimentally. Contrary to analog quantum simulation, the variational approach forgoes the requirement of realising the target Hamiltonian directly in the laboratory, thus allowing the study of a wider variety of previously intractable target models experimentally (including universal penalty functions [16]). This comes at the cost of increased measurements and classical pre- and postprocessing.

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 [20]. As the authors [20] 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 [21]. Their ansatz was of modified checkerboard form.
3. VQE (lattice simulation). Self-verifying variational algorithms as proposed in [22] and elsewhere have vanishing objective functions when the solution is reached. Such an approach was used in [22] to simulate the ground state of the lattice Schwinger model using 8 qubits realized by trapped ions.

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 (see the popular summary of the topic [4]). Quantum supremacy has also recently been experimentally demonstrated [3], which enables certain variational quantum algorithms [20; 21].

The validity of the results confirmed by consistency with prior art

Results forming this Habilitation thesis 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, as introduced partly in [23; 24], was formally proven (in the noise free setting) to represent a universal model of quantum computation by the author in [16]. 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.

Little is known about the ultimate practical capacity of the variational model in practice: present tools are difficult to apply to this new framework. Interesting recent findings include the discovery of barren plateaus [25] and (together with coauthors) of reachability deficits [17], a recent connection between variational algorithms and contextuality has been made in [26], and novel findings relating barren plateaus to circuit depth appeared in [27]. The finding of reachability deficits showed that existing papers applying QAOA are all too often in a low density subset of the possible problem instances. Hence, representative examples were not considered, which avoided these deficits. The result is entirely consistent with the state of the art in the topic.

As variational quantum algorithms rely on minimization of some cost function, an important finding shows how to evaluate the gradients of said cost function exactly [28; 29]. In addition, less general, though equally interesting work includes studying level-1 QAOA [30] and recent findings related to circuit-parameter concentrations between instance solutions [31]. The topic is developing rapidly. It is already large enough where a single thesis can not cover all of the developments. However, the core and central ideas are covered here. These ideas (as developed by many researchers over many years) have remained central to my research. The foundations are certainly covered here with the main and essential findings outlined in what I hope is an expository fashion.

Presentation of thesis contents

Contents and results from this thesis were presented by the author to peers at the following scientific events.

1. **Variational Models of Quantum Computation**
   Episode IX, Google Research Series on Quantum Computing
   Google Poland, Warsaw Poland, 10 October 2019
   Invited Research Lecture[2]

2. **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
   Invited Research Lecture[3]

3. **Quantum Enhanced Machine Learning**
   Physics Challenges in Machine Learning for Network Science
   Queen Mary University of London
   London, United Kingdom, September 2019
   Invited Research Lecture[4]

4. **Quantum Machine Learning for Quantum Simulation**
   Machine Learning for Quantum Matter
   Nodita, Stockholm, Sweden, August 2019
   Invited Research Lecture[5]

5. **Recent Results in the Theory of Variational Quantum Computation**
   the 5th International Conference on Quantum Technologies

[2] Video URL. https://www.youtube.com/watch?v=P52iqU50NHg
[3] Video URL. https://www.purdue.edu/data-science/quantum-machine-learning/
[4] Video URL. https://www.qmul.ac.uk/maths/news-and-events/events-/physics-challenges-for-machine-learning-and-network-science/
[5] Video URL. https://indico.fysik.su.se/event/5644/

The Russian Quantum Center, Moscow Russia 2019
Invited Research Lecture[6]

6. **Variational Quantum Computation in Photonics**
   The 28th Annual International Laser Physics Workshop
   Gyeongju, South Korea
   Invited Research Lecture

7. **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)

8. **Quantum Machine Learning Matrix Product States**
   Keynote talk at the Workshop on Quantum Information
   Harvard, USA, April 23-24, 2018

9. **Quantum Complex Networks**
   Keynote Lighting Talk at International school and conference on network science (NetSci)
   Paris, France 2018

The author's professional impact short summary

The author is an Associate Professor at the Skolkovo Institute of Physics and Technology and the Head of the Institutes Laboratory for Quantum Information Processing.

As is part of the Russian standard (at least in recent times), impact summaries are typically quantified with citation counts. As of May 2020, mine are as follows.

[6]Video URL. http://conference.rqc.ru

1. ORCHID ID https://orcid.org/0000-0002-0590-3327
2. Entries appearing in ORCHID 80
3. Total citations[7] 3,834
4. Total citations in prior year (2019) 849
5. h-index 27
6. i10-index 42
7. Papers in Web of Science top 1% highly cited papers index: 3
8. Papers in Web of Science top 0.1% highly cited papers index: 1

List of relevant publications

The author confirms their significant (or sometimes sole) involvement in the design and execution of the research published in the following peer reviewed works.

Furthermore, the author asserts that these publications were not used as part of any other degree.

Selected primary research articles related to the thesis 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.
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[7] Data collected from Google Scholar on September 2020.

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Books related to the thesis contents

1. Biamonte J. Lectures on Quantum Tensor Networks // arXiv:1912.10049 [cond-mat, physics:math-ph, physics:quant-ph]. 2020.
2. Baez J., Biamonte J.D. Quantum Techniques in Stochastic Mechanics. WORLD SCIENTIFIC, 2018.

Review articles related to the thesis contents

1. Biamonte J., Bergholm V. Tensor Networks in a Nutshell // arXiv:1708.00006 [cond-mat, physics:gr-qc, physics:hep-th, physics:math-ph, physics:quant-ph]. 2017.
2. Biamonte J., Faccin M., De Domenico M. Complex networks from classical to quantum // Commun Phys. 2019. Vol. 2, № 1. P. 53.
3. Biamonte J. et al. Quantum Machine Learning // Nature. 2017. Vol. 549, № 7671. P. 195–202.

Selected experimental collaborations related to thesis contents

1. Palmieri A.M. et al. Experimental neural network enhanced quantum tomography // npj Quantum Inf. 2020. Vol. 6, № 1. P. 20.
2. Lu D. et al. Chiral quantum walks // Physical Review A. 2016. Vol. 93, № 4.
3. Wang Y. et al. Quantum Simulation of Helium Hydride Cation in a Solid-State Spin Register // ACS Nano. 2015. Vol. 9, № 8. P. 7769–7774.
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Brief chapter descriptions

The objective of this thesis has been to pull a thread through the various subjects that have culminated in the modern theory of quantum algorithms.

At the core of these concepts is the LOCAL HAMILTONIAN problem. We considered several variants throughout the text.

The early chapter (§ 1) presented results which would enable one to sculpt Hamiltonians. This was done by mapping generalized Ising models between pseudo Boolean functions. A variety of algebraic tools exist to minimize and manipulate pseudo Boolean and Boolean functions. Particularly to transform a k-body Hamiltonian into a 2-body one. My own contributions to programming diagonal ground states appears in [7] as well as in joint work [8; 19]. Several evident Hamiltonain problems were connected to the theory of computational complexity theory.

The early chapter also presented some interesting findings [10] which relate physical and computational complexity. Indeed, we showed that the computational phase transition signature can be physically observed through Gibbs sampling [10]. This is indeed relevant to current experimental demonstrations and it is the subject of ongoing work to experimentally demonstrate our numerical simulations.

The next chapter (§ 2) presented a comparison between stochastic and quantum mechanics in several capacities. This comparison is central to my own research as well as ample contemporary studies. The approach I have taken, with several coauthors, is to establish a comparison inside the language of quantum walks. Every quantum process admits a quantum walk in the single particle basis, so the model is rather general. Joint work on this topic centers around [11; 32–36] subsequently surveyed in [11]. § 2 concludes by focusing on a comparison between the quantum and stochastic ground state energy problems.

Setting the stage for work to come and also presenting a few results, § 3 presents tensor networks as well as their relationship with quantum circuits. The presented results include presenting the minimal generators of stabilizer tensor networks (Theorem 11). This proof appeared in my paper [37]. The main result of the section was a graphical proof of the Gottesman–Knill Theorem (see Theorem 12). I am not aware of such a result being previously published though the result is not extremely surprising based on the capacity of the known graphical languages.

Next § 4 begins by applying circuits (as a variational ansatz) to approximate optimization problems. The chapter defines some of the necessary complexity theory background. Then importantly, the variational model of quantum computation is defined rather precisely, following my work in [16]. The start of the chapter also follows partially the results from the collaboration published as [13].

An old problem of importance is how to realize controlled unitary gates as a sequence of two-body gates. The chapter presents a factorization that was inspired by work appearing in the book [14]. With some small but notable improvements, herein we present a competitive method to realize such gates. We quantify the scaling of the method exactly. I am unaware of such a result being previously published.

Towards our goals, we have included a derivation showing that reasonable depth circuits can saturate bipartite entanglement—the depth of these circuits scales with the number of qubits and also depends on the interaction geometry present in a given quantum processor. This result follows my work [16] as well as the collaboration [15] and establishes a relationship between an objective circuit (to be simulated) and a given ansatz state.

Finally, § 4 concludes with recalling a fundamental limitation discovered in [17] with coauthors. The QAOA algorithms that exploit variational state preparation to find approximate ground states of Hamiltonians encoding combinatorial optimization problems. In particular we consider the Quantum Aproximate Optimization Algorithm or QAOA [24]. As a means to study the performance of QAOA, we turn to constraint satifiability—a tool with a successful history which was covered in detail in § 1 (see particularly § 1.5). Such problems are expressed in terms of N variables and M clauses (or constraints). Interesting, we found that the problems density strongly correlates with the ability of QAOA to solve a specific problem instance.

Going further than § 4, next § 5 followed the results in [16] and presented universal penalty functions for variational quantum computation. The presented penalty functions are formally proven to have a number of desirable qualities. The objective was to simulate the output of an L gate quantum circuit acting on the n-qubit product state $|0\rangle^{\otimes n}$. We have defined an objective function that when minimized will produce a state close to the desired quantum circuit output.

We then conclude the presentation of research in § 6 by covering several results, many of which are widely used that came primarily out of the work [18; 19]. The YY gadget in particular was derived by Yudong Cao. I attempted the same calculation but stopped after asymmetry caused terms to cancel. We decided to take the calculation one order further, lead by Yudong. He hence recovered the desired coupling and we worked together to dress the terms and minimize the error.

In closing, this thesis set out to carve a path through the core area of research related to contemporary quantum programming. Many of the results presented played their own role in developing the field we have arrived at today, which is dominated by variational algorithms. Having spent a number of years working on the topic, I found it tantalizing to be able to paint this picture and show some relationships between all of these contemporarily relevant topics. I hope future readers will indeed find the presentation and explanations, when given, to be of additional value. There are also a few unpublished results scattered around these pages that might one day become parts of research papers.

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