

---

---

# Quantum algorithms for Hamiltonian learning problems

---

---

*A thesis submitted in fulfilment of the requirements  
for the degree of*

Doctor of Philosophy

*in*

Computer Science (Quantum Computing)

*by*

Youle Wang

*to*

Centre for Quantum Software and Information, School of Computer  
Science

Faculty of Engineering and Information Technology

University of Technology Sydney

NSW - 2007, Australia

November 24, 2022



## CERTIFICATE OF ORIGINAL AUTHORSHIP

I, Youle Wang, declare that this thesis is submitted in fulfilment of the requirements for the award of Doctor of Philosophy, in the School of Computer Science, Faculty of Engineering and Information Technology at the University of Technology Sydney.

This thesis is wholly my own work unless otherwise referenced or acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis.

This document has not been submitted for qualifications at any other academic institution.

This research is supported by the Australian Government Research Training Program.

**Signature:** Production Note:  
Signature removed prior to publication.

**Date:** July 2022



## ABSTRACT

Learning the dynamic Hamiltonian of a quantum system is a fundamental task in studying condensed matter physics and verifying quantum technologies. Many protocols have been proposed for Hamiltonian learning. Still, many of them require the ability to prepare quantum Gibbs states and estimate entropies of quantum states, which are not easy for classical computers. Recent experimental progress of quantum hardware has drawn much attention, motivating us to investigate the application of near-term quantum computers in Hamiltonian learning. In this dissertation, we study the Hamiltonian learning problems and propose algorithms to recover interaction coefficients of a Hamiltonian, prepare quantum Gibbs states, and estimate the quantum entropies of quantum states. We employ quantum circuits that are expected to be implementable in the near-to-intermediate future.

First, we use the variational quantum algorithms to enable a hybrid quantum-classical algorithmic scheme to tackle the Hamiltonian learning problem. By transforming the Hamiltonian learning problem to an optimization problem using the Jaynes' principle, we employ a gradient-descent method to give the solution and could reveal the interaction coefficients from the system's Gibbs state measurement results. In particular, the computation of the gradients relies on the Hamiltonian spectrum and the log-partition function. Hence, as the main subroutine, we develop a variational quantum algorithm to extract the Hamiltonian spectrum and utilize convex optimization to compute the log-partition function. We also apply the importance sampling technique to circumvent the resource requirements for large-scale Hamiltonians.

Second, we propose variational quantum algorithms for quantum Gibbs state preparation. First, we take the loss function as the system's free energy and estimate it by a truncated version. Then we train a parameterized quantum circuit to optimize the loss function so that it can learn the desired quantum Gibbs state. Notably, our algorithms can be implemented on near-term quantum computers. Furthermore, by performing numerical experiments, we show that shallow parameterized circuits with only one additional qubit can be trained to prepare the Ising chain and spin chain Gibbs states with a fidelity higher than 95%. In particular, for the Ising chain model, we find that a simplified circuit ansatz with only one parameter and one additional qubit can be trained to realize a 99% fidelity in Gibbs state preparation at inverse temperatures larger than 2.

Third, we propose quantum algorithms to estimate the von Neumann and quantum  $\alpha$ -Rényi entropies of an  $n$ -qubit quantum state  $\rho$  using independent copies of the input

---

state. We show how to efficiently construct the quantum circuits of both methods using primitive single/two-qubit gates. We prove that the number of required copies scales polynomially in  $1/\epsilon$  and  $1/\Lambda$ , where  $\epsilon$  denotes the additive precision and  $\Lambda$  denotes the lower bound on all non-zero eigenvalues. Notably, our method outperforms previous methods in the aspect of practicality since it does not require any quantum query oracles, which are usually necessary for previous methods. Furthermore, we conduct experiments to show the efficacy of our algorithms to single-qubit states and study the noise robustness.

## DEDICATION

*To my family.*





## STATEMENT OF AUTHORSHIP AND PUBLICATIONS

The dissertation is based on the following articles:

- Youle Wang, Guangxi Li, and Xin Wang. A hybrid quantum-classical Hamiltonian learning algorithm. *Sci. China Inf. Sci.* 66, 129502 (2023). <https://doi.org/10.1007/s11432-021-3382-2>
- Youle Wang, Guangxi Li, and Xin Wang. (2020). Variational quantum Gibbs state preparation with a truncated Taylor series. *Physical Review Applied*, 16(5), 054035. <https://doi.org/10.1103/PhysRevApplied.16.054035>
- Youle Wang, Benchu Zhao, and Xin Wang. (2022). Quantum algorithms for estimating quantum entropies. <http://arxiv.org/abs/2203.02386>

The first work above has been published in *Science China Information Sciences* and was also accepted as a short talk at the 21st Asian Quantum Information Science Conference, AQIS 2021. The second work has been published in *Physical Review Applied*. The third work is available online. In addition, I have co-authored the following articles that are not included in this dissertation. In the first work below, the authors are listed in alphabetical order.

- Xin Wang, Youle Wang, Zhan Yu, and Lei Zhang. Quantum Phase Processing: Transform and Extract Eigen-Information of Quantum Systems. <http://arxiv.org/abs/2209.14278>
- Xin Wang, Zhixin Song, and Youle Wang. (2021). Variational Quantum Singular Value Decomposition. *Quantum*, 5(1), 483. <https://doi.org/10.22331/q-2021-06-29-483>
- Guangxi Li, Youle Wang, Yu Luo, Yuan Feng, Quantum data fitting algorithm for non-sparse matrices. <http://arxiv.org/abs/1907.06949>

All my publications are available on arXiv and Google Scholar.



## ACKNOWLEDGMENTS

This dissertation would not have been possible without the support I received during the doctoral study. I express my sincere gratitude and appreciation to all people who have helped me.

First, I want to thank my supervisor, professor Yuan Feng, who introduced me to quantum computing and taught me how to do research at the beginning of my research journey. In each meeting, he would listen carefully to my presentation and taught me how to make myself clear. His high research standards and profound knowledge in the area impressed me. I also sincerely thank him for giving me the freedom to communicate with other researchers and the support to visit overseas. In particular, I appreciate his support during the great pandemic of COVID-19.

I am very grateful to professor Sanjiang Li and professor Zhengfeng Ji for guiding my study. Sanjiang Li has provided much kind advice for me in research and life and is also very nice. Zhengfeng is a very expert in the area and has a very high taste for research. When I was wandering at the beginning of my study, Zhengfeng shared his experience in research to guide me through the time. And he would share his opinion about the research I focused on and push me to study further to deepen my understanding and do more meaningful research.

Moreover, I thank the partners and friends from Institute for Quantum Computing, Baidu, where I have had a great time and done much interesting research. I thank Institute for Quantum Computing, Baidu, for giving me the opportunity to join them as visiting student and research intern during my studies. I thank mentor Xin Wang for leading me to research projects during my internship. I am deeply inspired by his expertise in the area and the rigour he pursues in research, from which I can benefit a lot. I also appreciate him and Lijing Jin for hosting a birthday party.

During the visiting at Baidu, I had met many friends with diverse backgrounds. Their diverse research backgrounds and expertise have brought many meaningful discussions and collaborations. I cherish the opportunities to work Zhixin Song, Ranyiliu Chen, and Benchu Zhao and thank them for sharing their knowledge in different areas. I also have enjoyed in-depth discussions with many interns, including Xuanqiang Zhao, Zihe Wang, Xia Liu, Chengkai Zhu, Chenfeng Cao, Jiaqing Jiang, Sizhuo Yu, Kaiyan Shi, Zihan Xia, and many others not mentioned. I thank them for sharing their knowledge and perceptive opinions.

Finally, I thank my friends and colleagues at UTS: Ji Guan, Guangxi Li, Yu Luo, and Xiangzhen Zhou. When I first arrived in Sydney, Ji Guan helped me settle down. I

---

learned a lot from him about living in a foreign country. Guangxi Li is very expertise in computers, and he taught me a lot about programming. Yu Luo is very smart and patient. We often worked together to solve complex mathematical questions. Xiangzhen Zhou is a great friend and roommate. He also is a devout Christian. He often drove me to the Church on Sunday, where I learned about church and belief. We shared an apartment for one year, which was a great time, and I miss it. In particular, I thank my family for the endless love and support for allowing me to pursue my dreams.

# TABLE OF CONTENTS

<b>List of Figures</b>	<b>xiii</b>
<b>List of Tables</b>	<b>xvii</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Hamiltonian learning . . . . .	1
1.2 Quantum Gibbs state preparation . . . . .	3
1.3 Quantum entropy estimation . . . . .	4
<b>2 Preliminary</b>	<b>7</b>
2.1 Notation and terminology . . . . .	7
2.2 Variational quantum algorithms . . . . .	8
2.2.1 Parameterized quantum circuit . . . . .	8
2.2.2 Variational quantum eigensolver . . . . .	8
2.2.3 Gradient estimation . . . . .	9
<b>3 Quantum Hamiltonian learning algorithm</b>	<b>11</b>
3.1 Problem Statement . . . . .	11
3.2 A gradient-descent solution . . . . .	13
3.3 Hamiltonian learning algorithm . . . . .	17
3.3.1 Variational quantum Hamiltonian spectrum solver . . . . .	18
3.3.2 Gradient estimation . . . . .	21
3.4 Numerical Results . . . . .	23
3.4.1 Random Hamiltonian models . . . . .	23
3.4.2 Quantum many-body models . . . . .	25
3.4.3 Numerical results using fewer eigenvalues of Ising Hamiltonians . . . . .	26
<b>4 Quantum Gibbs state preparation</b>	<b>31</b>
4.1 Loss function . . . . .	31

## TABLE OF CONTENTS

---

4.2	Variational quantum Gibbs state preparation . . . . .	33
4.3	Error analysis . . . . .	35
4.4	Gradient . . . . .	40
4.5	Numerical results . . . . .	44
4.5.1	Ising model . . . . .	44
4.5.2	XY spin-1/2 chain model . . . . .	49
<b>5</b>	<b>Quantum entropy estimation</b>	<b>53</b>
5.1	Quantum entropy approximations . . . . .	54
5.1.1	Approximation of von Neumann entropy . . . . .	54
5.1.2	Approximation of $\alpha$ -Rényi entropy . . . . .	59
5.1.3	Approximation error analysis . . . . .	66
5.2	Quantum circuit construction . . . . .	67
5.2.1	Circuit scheme . . . . .	67
5.2.2	Circuit width circumvent . . . . .	70
5.2.3	A subroutine . . . . .	71
5.3	Quantum entropy estimation . . . . .	74
5.4	Numerical results . . . . .	81
5.4.1	Effectiveness and correctness . . . . .	81
5.4.2	Robustness . . . . .	82
5.5	Comparison to literature . . . . .	85
5.6	Applications . . . . .	85
<b>6</b>	<b>Conclusion and future work</b>	<b>87</b>
<b>A</b>	<b>Appendix</b>	<b>91</b>
A.1	Supplementary proofs . . . . .	91
A.2	Variational algorithm for Gibbs state preparation with higher-order truncations . . . . .	99
A.3	Estimation of the higher-order gradients . . . . .	99
A.4	Supplementary discussion for optimization . . . . .	101
A.5	Gate decomposition . . . . .	103
A.6	Barren plateaus . . . . .	103
	<b>Bibliography</b>	<b>109</b>

## LIST OF FIGURES

FIGURE	Page
2.1 A circuit module of PQC. $U_l(\theta_l)$ is a gate with tunable parameter $\theta_l$ , and $W_l$ is a parameter-free gate, e.g., CNOT. . . . .	9
3.1 Flowchart of the gradient-descent method for Hamiltonian learning. . . . .	13
3.2 The selected quantum circuit $U(\boldsymbol{\theta})$ for stochastic variational quantum eigensolver (SVQE). Here, $D$ represents circuit depth. Parameters $\boldsymbol{\theta}$ are randomly initialized from a uniform distribution in $[0, 2\pi]$ and updated via gradient descent method. . . . .	24
3.3 The curves in (a), (b), (c) represent the infinity norm of the error of $\mu$ with different $\beta$ , different number of $\mu$ , and different number of qubits, respectively. In (d), (e), (f), the curves represent the infinity norm of the error of $\mu$ for different many-body Hamiltonians with the number of qubits varies from 3 to 5. The numbers on the line represent the values of the last iteration. These numbers close to 0 indicate that our algorithm is effective. . . . .	28
3.4 Experimental results by using fewer eigenvalues. Each line corresponds to the results by running HQHL with Ising Hamiltonians of different sizes. Results show that using halved circuit depth, compared to the setting in Sec. 3.4.2, could learn coefficients up to precision 0.05 for different sized Ising models and a different number of $\mu$ . . . . .	29
4.1 Quantum circuit for implementing Destructive Swap Test. In the circuit, two states $\rho$ and $\sigma$ are prepared at different registers. Then CNOT and Hadamard gates are performed as shown. The state overlap can be estimated via post-processing. . . . .	32

4.2 Quantum circuit for computing  $\text{tr}(\rho^3)$ . In the circuit, the  $U(\theta)$  denotes the state preparation circuit, and  $H$  denotes the Hadamard gate. Four registers are used to prepare states by  $U(\theta)$ , and one ancillary qubit is used to perform the controlled swap operator. The qubit reset occurs on the bottom two registers, where the break in the wire means the reset operation. Notably, the state on the bottom two registers are first implemented with a circuit  $U(\theta)$  and controlled swap operator and then reset to state  $|0\rangle$ . Again,  $U(\theta)$  and controlled swap operator are performed on the bottom registers. Finally,  $\text{tr}(\rho^3)$  can be obtained via post-processing the measurement results. . . . . 32

4.3 Schematic representation of the variational quantum Gibbs state preparation with truncation order 2. First, we prepare the Hamiltonian  $H$  and inverse temperature  $\beta$  and then send them into the Hybrid Optimization. Second, we choose an ansatz and employ it to evaluate the loss function  $L_1, L_2, L_3$  on quantum devices. Then we calculate the difference  $\Delta\mathcal{F}_2(\theta)$  by using  $L_1, L_2, L_3$ . Next, if the condition  $\Delta\mathcal{F}_2 \leq \epsilon$  is not satisfied, then we perform classical optimization to update parameters  $\theta$  of the ansatz and return to the loss evaluation. Otherwise, we output the current parameters  $\theta^*$ , which could be used to prepare Gibbs state  $\rho_G$  via  $U(\theta)$ . Here in the quantum device, registers  $A_2, B_2, A_3, B_3$  are used to evaluate  $\text{tr}(\rho_{B_2}\rho_{B_3})$  and registers  $A_4, B_4, \dots, A_6, B_6$  are used to evaluate  $\text{tr}(\rho_{B_4}\rho_{B_5}\rho_{B_6})$ . . . . . 34

4.4 Two ansatzes for Ising chain model. These ansatzes are composed of two registers  $A$  and  $B$ , where one ancillary qubit is set in  $A$  and 5 qubits are set in  $B$ . Notably, the qubits in  $B$  are performed with rotations  $R_y(\theta)$  and CNOT gates in (a), while only CNOT gates in (b). . . . . 42

4.5 Fidelity curves for the Ising chain Gibbs state preparation with different  $\beta$ . In (a), we use the Ansatz with 6 parameters (cf. Fig. 4.4(a)); In (b), we use the Ansatz with only 1 parameter (cf. Fig. 4.4(b)). We can see that they have almost the same performance, which indicates only 1 parameter is enough for this task. . . . . 43

4.6 Semilog plot of the fidelity vs. the Ising Hamiltonian length ( $L$ ) with different  $\beta$  for the Ising chain model. Here,  $\log_2$  means logarithm with base 2. We can see that the fidelity increases exponentially with  $\beta$  growing. . . . . 43



4.7 The ansatz for XY spin-1/2 chain model. In this ansatz, it contains one ancilla qubit in register  $A$  and 5 qubits in register  $B$ . Rotation gates  $R_y(\theta)$  are first applied on all qubits. Then, a basic circuit module (denoted in the dashed-line box) composed of CNOT gates and rotation gates  $R_y(\theta)$  is repeatedly applied. Here,  $d$  means repeating  $d$  times. . . . . 49

4.8 Fidelity curves for the XY spin-1/2 chain Gibbs state preparation with different  $\beta$ . The results of the fidelity obtained with different  $\beta$  are represented by coloured lines. In (a)-(d), numerical experiments are performed using different ansatzes. In each ansatz, the basic circuit module (cf. Fig. 4.7) is repeated different times, i.e.,  $d$ . Note that each ansatz has  $(n_A + n_B)(d + 1) = 6(d + 1)$  parameters. Here better performance are obtained with larger  $d$ . . . . . 50

4.9 Boxplot of the fidelity vs. the truncation order  $K$  with different  $\beta$  for the XY spin-1/2 chain model. Here the ansatz is similar to Fig. 4.7 while  $n_A = n_B = 3$ . Each box consists of 30 runs with different parameter initializations. . . . . 51

5.1 For a short time  $t$ , we first prepare a ground state  $|0\rangle\langle 0|$  in the measure register, and prepare states  $\rho$  in the main register the ancillary register, respectively. Subsequently, perform the controlled unitary operator  $e^{-i\mathcal{S}t}$  on state  $\rho \otimes \rho$ . At the end of the circuit, we measure along the eigenbasis of Pauli  $Z$ , which would immediately lead to an estimate for  $\text{tr}(\rho \cos(\rho t))$  up to precision  $O(t^2)$ . . . . . 68

5.2 For general time  $t$ , the circuit could be inductively constructed. The operator  $e^{-i\mathcal{S}\Delta t}$  is sequentially applied on the main register and different ancillary registers, conditional on the measure register. Here, we append  $Q$  ancillary states and use  $Q$  times of  $e^{-i\mathcal{S}\Delta t}$ . For clear, we label states on different register by  $1, 2, 3, Q + 1$ , and the script of the swap operator indicates the registers that swap operator acts on. . . . . 69

5.3 A quantum circuit for estimating  $\text{tr}(\rho \cos(\rho t))$  using qubit reset. The break and a state  $\rho$  in the wire means implementing qubit reset. . . . . 71

5.4 Quantum circuit for implementing the module  $W$ . . . . . 72

5.5 This figure depicts the resulting circuit by substituting  $c-e^{-iS\Delta t}$  with the circuit of controlled-A (dashed box) in Figure 5.1. The dotted circuit is the controlled-W circuit, in which the  $c-R_1$  and  $oc-R_2$  are the 1-controlled  $R_1$  gate (apply  $R_1$  on the target qubit if the control qubit in state  $|1\rangle$ ) and 0-controlled  $R_2$  gate (apply  $R_2$  on the target qubit if the control qubit in state  $|0\rangle$ ), respectively. The definitions of  $R_1$  &  $R_2$  can be found in Eqs. (5.113)-(5.114). The circuits between dotted boxes are known as reflectors. Denote that all elements in the circuit can be broken down into single/two-qubits gates, please refer to Appendix A.5 for details. . . . . 73

5.6 In (a) and (b), the black dashed line represents the actual entropy of quantum state  $\rho$ . The blue and orange curves are average entropy over 20 repeats for  $\epsilon$  equal to 0.2 and 0.4, respectively. The shadowed area stands for standard deviation. . . . . 82

5.7 The results for 4 randomly generated states. In (a) and (b), the blue bar is the real quantum entropy, the Estimated Entropy 1 stands for the entropy corresponding to the Fourier series approximation, and the Estimated Entropy 2 is the average entropy (100 sample points, repeat 20 times) calculated by our approach. In addition, the error bar represents the standard deviation. . . . . 83

5.8 Figures (a) and (b) represent results for von Neumann entropy, and (c) and (d) represent the results for 2-Rényi entropy. The green curves link the average estimated entropy at different noise levels. The black dashed line represents the actual von Neumann entropy of quantum state  $\rho$ . . . . . 84

A.1 Quantum circuit for anti-controlled rotation  $oc-R_2$ . . . . . 103

A.2 Quantum circuit for controlled phase gate  $c-S$ . . . . . 103

A.3 Quantum circuit for implementing controlled  $select(S)$ . Here we take three-qubit state  $\rho$  as example. The circuit appends one qubit  $|0\rangle$ . The decomposition of the  $c-S$  is given in Figure A.2. Particularly, the  $c-Z$  gate is applied only when  $t > 0$ . . . . . 104

## LIST OF TABLES

TABLE	Page
<p>3.1 Hyper-parameters setting. The number of qubits (# qubits) varies from 3 to 5, and the number of <math>\mu</math> (# <math>\mu</math>) from 3 to 6. <math>\beta</math> is chosen as 0.3, 1, 3. “LR” denotes learning rate. The values of <math>\mu</math> are sampled uniformly in the range of <math>[-1, 1]</math>. The term, likes “[0 2 1] [2 1 3] [0 3 3]”, indicates there are three <math>E_i</math>’s and each has three qubits with the corresponding Pauli tensor product. Here “0,1,2,3” represent “<math>I, X, Y, Z</math>” respectively. For example, for the first sample, the corresponding Hamiltonian is taken as <math>H=0.3408 \cdot I \otimes Y \otimes X - 0.6384 \cdot Y \otimes X \otimes Z - 0.4988 \cdot I \otimes Z \otimes Z</math>. . . . .</p>	24
<p>3.2 Hyper-parameters setting for many-body models. For each Hamiltonian model, the number of qubits varies from 3 to 5, and the number of <math>\mu</math> is determined by the number of Pauli operators. “LR” denotes learning rate. The values of <math>\mu</math> are sampled uniformly in the range of <math>[-1, 1]</math>. . . . .</p>	25
<p>3.3 Parameters setting for HQHL. The script index means the length of the tuple, e.g., <math>()_8</math> indicates the tuple consists of 8 entries. The notation <math>0, \dots</math> means the entries following 0 are all zeros as well. Notation <math>\#\lambda</math> means the number of eigenvalues we learned. Please note that we omit the <math>\beta = 1</math> in the table. . . . .</p>	27
<p>5.1 Upper bound on the overall weights. . . . .</p>	64
<p>5.2 Cost estimation of Algorithm 7 . . . . .</p>	78

