



Universiteit
Leiden
The Netherlands

Optimization of quantum algorithms for near-term quantum computers

Bonet Monroig, X.

Citation

Bonet Monroig, X. (2022, November 2). *Optimization of quantum algorithms for near-term quantum computers. Casimir PhD Series*. Retrieved from <https://hdl.handle.net/1887/3485163>

Version: Publisher's Version

License: [Licence agreement concerning inclusion of doctoral thesis in the Institutional Repository of the University of Leiden](#)

Downloaded from: <https://hdl.handle.net/1887/3485163>

Note: To cite this publication please use the final published version (if applicable).

Optimization of quantum algorithms for near-term quantum computers

PROEFSCHRIFT

TER VERKRIJGING VAN
DE GRAAD VAN DOCTOR AAN DE UNIVERSITEIT LEIDEN,
OP GEZAG VAN RECTOR MAGNIFICUS PROF. DR. IR. H. BIJL,
VOLGENS BESLUIT VAN HET COLLEGE VOOR PROMOTIES
TE VERDEDIGEN OP WOENSDAG 2 NOVEMBER 2022
KLOKKE 15.00 UUR

DOOR

Xavier Bonet-Monroig

GEBOREN TE XÀTIVA, VALÈNCIA (SPANJE)
IN 1991

Promotor: Prof. dr. C. W. J. Beenakker
Co-promotor: Dr. T. E. O'Brien
Promotiecommissie: Prof. dr. A. Montanaro (University of Bristol)
Prof. dr. L. Visscher (Vrije Universiteit Amsterdam)
Prof. dr. J. Aarts
Prof. dr. A. Achúcarro
Dr. J. Tura i Brugués

Casimir PhD series, Delft-Leiden 2022-31

ISBN 978-90-8593-541-4

An electronic version of this thesis can be found
at <https://openaccess.leidenuniv.nl>

Cover: Two roses that arise from the same root are drawn using quantum gates. Inside them there are mathematical descriptions of quantum circuits. One of the roses has been carefully cared and has grown strong and with bright colors. It is a metaphorical representation of a quantum algorithm that has been successful, with errors fully mitigated. The other rose has not been carefully treated, it has not been able to grow and its colors are dull. It is a metaphorical description of a failed quantum algorithm because errors have not been properly mitigated. Illustration by Cristina Cejudo Vera.

To my family: Anna, Xavi and Ada, and to Mireia for always being there.

“There is a flower... I think she has tamed me...”
Antoine de Saint-Exupéry

Contents

1. Introduction	1
1.1. Preface	1
1.2. Basics of quantum algorithms	2
1.2.1. Quantum state tomography	3
1.2.2. Variational quantum algorithms	6
1.2.3. Classical optimization of variational quantum algorithms	8
1.2.4. Applications to quantum chemistry and material science	10
1.3. Noisy intermediate-scale quantum computers	12
1.3.1. Noise in quantum hardware	13
1.3.2. Quantum error correction	14
1.3.3. Quantum error mitigation	15
1.4. Outline of this thesis	16
2. Low-cost error mitigation by symmetry verification	19
2.1. Introduction	19
2.2. Symmetry verification	20
2.2.1. Ancilla and in-line symmetry verification	21
2.2.2. Variational quantum eigensolvers	22
2.2.3. Post-selected symmetry verification and S-QSE	26
2.3. Simulation of symmetry verification on the hydrogen molecule	28
2.4. Inserting and rotating symmetries	30
2.5. Extending the symmetry verification of the hydrogen molecule	34
2.6. Conclusion	37
2.A. Appendix: Error mitigation of QSE with anticommuting operators	39
3. Experimental error mitigation via symmetry verification in a variational quantum eigensolver	43
3.1. Introduction	43
3.2. Variational quantum eigensolvers for the Hydrogen molecule	44
3.3. Experimental error mitigation via symmetry verification	46
3.4. Effect of symmetry verification on positivity constrains	53

3.5. Conclusion	54
3.A. Appendix: Tomographic reconstruction and limitations . .	55
3.B. Appendix: Constraining the positivity of reduced density matrices	57
3.C. Appendix: Theoretical modeling of the experiment	57
3.C.1. Numerical simulations	57
3.C.2. Exchange gate	58
4. Nearly-optimal measurement scheduling for partial tomography of quantum states	61
4.1. Introduction	61
4.2. Background	64
4.3. Near-optimal measurement schemes for local qubit and fermion operators	65
4.4. Measuring anti-commuting linear combinations of local fermionic operators	69
4.5. Conclusion	69
4.A. Appendix: Schemes for partial state tomography of qubit k -RDMs	71
4.B. Appendix: Upper bounds on the size of commuting cliques of Majorana operators	73
4.C. Appendix: Details of measurement schemes for fermionic systems	75
4.D. Appendix: Reducing operator estimation over symmetries	78
4.E. Appendix: Parallel iteration over pairings	80
4.F. Appendix: Measurement circuitry for fermionic RDMs . .	81
4.G. Appendix: Proof that the maximum size of an anti-commuting clique of Pauli or Majorana operators is $2N+1$	83
4.H. Appendix: Proof of theorem 1	84
5. Performance comparison of optimization methods for variational quantum algorithms	87
5.1. Introduction	87
5.2. Background	88
5.3. Three-stage sampling adaptation	90
5.4. Hyperparameter tuning	93
5.5. The sampling noise floor	95
5.6. Conclusion	96
5.A. Appendix: Details on optimization algorithms	99
5.B. Appendix: Numerical experiments	100
5.C. Optimization algorithms hyper-parameters	102

5.D. Appendix: Unitary Coupled-Cluster ansatz based on coupled-cluster amplitudes	103
5.E. Appendix: Variational Hamiltonian ansatz for the Hubbard model	106
6. Quantum simulation of hydrogen molecule on Quantum Inspire	109
6.1. Introduction	109
6.2. Quantum simulation of the Hydrogen molecule	110
6.2.1. Variational quantum eigensolvers	110
6.2.2. Ground-state energy of the Hydrogen molecule via VQE	111
6.2.3. Implementation in Quantum Inspire	111
6.2.4. Results	113
6.3. Conclusion and outlook	115
7. Calculating energy derivatives for quantum chemistry on a quantum computer	119
7.1. Introduction	119
7.2. Background	120
7.3. The quantum chemical Hamiltonian	121
7.4. Energy derivative estimation using eigenstate truncation approximation	121
7.5. Geometry optimization on a superconducting quantum device	124
7.6. Polarizability estimation	128
7.7. Conclusion	129
7.A. Appendix: Classical computation	131
7.B. Appendix: Experimental methods	132
7.C. Appendix: Simulation methods	133
7.D. Appendix: Numerical optimization and approximate Hessian calculations	133
Bibliography	137
Samenvatting	161
Summary	165
Resum	167
Curriculum Vitæ	171

Contents

List of publications

173