



Universiteit
Leiden
The Netherlands

The power of one qubit in quantum simulation algorithms

Polla, S.

Citation

Polla, S. (2024, February 22). *The power of one qubit in quantum simulation algorithms*. Casimir PhD Series. Retrieved from <https://hdl.handle.net/1887/3719849>

Version: Publisher's Version

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

License: <https://hdl.handle.net/1887/3719849>

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

The power of one qubit in quantum simulation algorithms

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 donderdag 22 februari 2024
klokke 15:00 uur

door

Stefano Polla

geboren te Bergamo, Italië
in 1994

Promotor: Prof. dr. C. W. J. Beenakker
Co-promotor: Dr. T. E. O'Brien

Promotiecommissie: Prof. Dr. J. Aarts
Dr. A. Roggero (Università di Trento)
Prof. Dr. K. E. Schalm
Prof. Dr. B. M. Terhal (Technische Universiteit Delft)
Prof. Dr. L. Visscher (Vrije Universiteit Amsterdam)

Casimir PhD series, Delft-Leiden 2023-42
ISBN 978-90-8593-587-2
An electronic version of this thesis can be found
at <https://openaccess.leidenuniv.nl>

On the cover: *an artistic representation of quantum computing emerging as a new technology, inspired by the rising cities painted by the futurist movement.* — by Jeanne M. Viet [Miss J Art]

To those who brightened my hardest days

Contents

1	Introduction	1
1.1	Preface	1
1.2	Processing quantum information	2
1.2.1	Classical input-output	3
1.2.2	Noise, error correction and mitigation	4
1.3	Targets of quantum simulation	6
1.3.1	Hamiltonian dynamics	8
1.3.2	State preparation	9
1.3.3	Energy measurements	11
1.3.4	The ground state energy problem	12
1.4	Algorithms for quantum simulation	13
1.4.1	Classical algorithms	13
1.4.2	Hamiltonian simulation algorithms	15
1.4.3	Adiabatic state preparation	16
1.4.4	The variational quantum eigensolver	18
1.4.5	Quantum phase estimation algorithms	19
1.5	Molecular simulation on a quantum computer	22
1.5.1	The pipeline for electronic structure on a quantum computer	23
1.5.2	The journey towards useful quantum advantage in chemistry	29
1.6	Outline of this thesis	31

Contents

2 Quantum digital cooling	35
2.1 Introduction	35
2.2 Cooling a system with a single fridge qubit	37
2.3 De-exciting a single transition: the 1+1 model	38
2.3.1 Elementary approaches to digital cooling: strong and weak coupling	39
2.3.2 Common symmetries and the coupling alternation method	42
2.4 Scalable QDC protocols	44
2.4.1 The BangBang protocol	44
2.4.2 The LogSweep protocol	47
2.5 Conclusion	54
Appendices	56
2.A Proof of Eq. (2.10)	56
2.B Asymptotic reheating and cooling probabilities for QDC protocols	57
2.C Optimizing energy spacing in LogSweep protocol	61
2.D Cooling rate for LogSweep protocol in a large system	61
2.E Effect of banding on QDC protocols	63
2.F Details on numerical methods	64
3 Error mitigation via verified phase estimation	67
3.1 Introduction	67
3.2 Pedagogical example of verification protocol for expectation value estimation	70
3.3 Schemes for verified phase estimation	73
3.3.1 Review of single-control quantum phase estimation	73
3.3.2 Verifying a phase estimation experiment	76
3.3.3 Why verification mitigates errors	78
3.3.4 Verified control-free phase-estimation	83
3.4 Verified expectation value estimation	85
3.4.1 Fast-forwarded and parallelized Hamiltonian decom- positions	88
3.4.2 Comparison to other methods of error mitigation	89
3.5 Numerical Experiments	92
3.5.1 Givens rotation circuits for free-fermion Hamiltonians	93
3.5.2 The variational Hamiltonian ansatz for the transverse- field Ising model	97
3.5.3 Fermionic swap networks for electronic structure Hamiltonians	98
3.5.4 Sampling costs	102

3.6	Conclusion	103
	Appendices	105
3.A	Error analysis	105
3.B	Effect of parallelizing QPE	110
3.C	Compensation for spurious eigenvalues due to sampling noise	113
3.D	Demonstration of immunity to control noise in single-control VPE	115
3.E	Use of a variational outer loop to mitigate constant unitary noise	115
3.F	Term-wise comparison of VPE performance	118
3.G	Comparison to symmetry verification	119
4	Optimizing the information extracted by a single qubit measurement	121
4.1	Introduction	121
4.2	Single-qubit measurements	122
4.2.1	The Hadamard test	123
4.2.2	Echo verification	125
4.2.3	Ancilla-free echo verification	126
4.2.4	Variance of a binary POVM	127
4.3	Operator decompositions	128
4.3.1	Adaptive shot allocation	129
4.3.2	The decomposition hierarchy	129
4.3.3	Optimizing reflection decompositions	131
4.3.4	Implementing the optimal decomposition	132
4.4	Numerical experiments	133
4.5	Conclusion	135
4.A	Echo verification estimators	136
4.B	Parallelizing echo verification	137
4.C	Proof of decomposition optimality hierarchy	139
4.C.1	Proof of Lemma 1, and corollaries	139
4.C.2	Proof of Lemma 2	141
4.C.3	Proof of Lemma 3	142
4.C.4	Examples of reflection decompositions	142
4.C.5	Proof of Lemma 4	144
4.D	Implementation of the Ξ decomposition via quantum signal processing	148
4.E	The generalized parameter-shift kernel decomposition of a diagonal operator with ladder spectrum	150
4.F	Details on numerical simulations and further numerical results	151

Contents

5 Virtual mitigation of coherent non-adiabatic transitions by echo verification	155
5.1 Introduction	155
5.2 The adiabatic algorithm and purification-based error mitigation	158
5.3 Mitigating coherent errors in adiabatic state preparation	159
5.4 Implementation and cost of the dephasing	161
5.5 Comparison with standard adiabatic algorithm.	162
5.6 Discussion and practical considerations.	163
5.A Dephasing operation on a degenerate spectrum	165
5.B Evaluation of AEV estimator with approximate dephasing	165
5.C Dephasing time for a smooth probability distribution	171
6 A hybrid quantum algorithm to detect conical intersections	175
6.1 Introduction	175
6.2 Background	177
6.2.1 Conical intersections	177
6.2.2 Berry phases in real Hamiltonians	179
6.2.3 Measuring Berry phase with a variational wavefunction	180
6.3 Methods	180
6.3.1 Fixing the gauge with a real ansatz	181
6.3.2 Avoiding full optimization via Newton-Raphson steps	182
6.3.3 Regularization and backtracking	183
6.3.4 Measuring the final overlap	185
6.3.5 Overview of the algorithm	186
6.4 Error analysis and bounding	188
6.4.1 Bounding the NR error	189
6.4.2 Bounding the sampling noise	190
6.4.3 Scaling of the total cost	191
6.5 Adapting to an orbital-optimized PQC ansatz	191
6.5.1 An OO-PQC ansatz with geometric continuity . .	192
6.5.2 Measuring boundary terms with the OO-PQC ansatz	193
6.5.3 Newton-Raphson updates of the OO-PQC ansatz .	194
6.6 Numerical results	195
6.6.1 Numerical simulation details	196
6.6.2 Minimal model with an degeneracy-free ansatz .	196
6.6.3 Sampling noise	198
6.6.4 Larger basis and active space	199
6.7 Conclusion and outlook	201
6.7.1 Paths towards improving convergence	202
6.7.2 Potential applications	204

6.7.3	Outlook	205
Appendices		206
6.A	Bounding overlaps by change in ansatz parameters	206
6.B	Bounding the norm of energy derivatives	208
6.C	Analytical orbital gradient and Hessian	209
6.D	Bounding the cumulative error due to Newton-Raphson updates	212
6.E	Bounding the sampling cost	216
Bibliography		219
Acknowledgments		243
Samenvatting		247
Summary		251
Sinossi		255
Curriculum Vitæ		259
List of publications		261