



Supercomputer simulations of transmon quantum computers

Dennis Willsch

IAS Series

Band / Volume 45

ISBN 978-3-95806-505-5

Mitglied der Helmholtz-Gemeinschaft

Forschungszentrum Jülich GmbH
Institute for Advanced Simulation (IAS)
Jülich Supercomputing Centre (JSC)

Supercomputer simulations of transmon quantum computers

Dennis Willsch

Schriften des Forschungszentrums Jülich
IAS Series

Band / Volume 45

ISSN 1868-8489

ISBN 978-3-95806-505-5

Contents

| | | |
|----------|---|-----------|
| 1 | Introduction | 1 |
| 2 | Ideal gate-based quantum computing | 5 |
| 2.1 | Quantum bits | 5 |
| 2.1.1 | Single qubits | 6 |
| 2.1.2 | Bloch sphere | 6 |
| 2.1.3 | Multiple qubits | 8 |
| 2.1.4 | Leakage | 11 |
| 2.2 | Quantum gates | 12 |
| 2.2.1 | Unitary operators | 12 |
| 2.2.2 | Elementary quantum gates | 13 |
| 2.3 | Quantum circuits | 14 |
| 2.4 | Quantum operations | 16 |
| 2.4.1 | Representations of quantum operations | 17 |
| 2.4.2 | Transformations of subsystems and leakage | 19 |
| 3 | Simulating superconducting transmon qubits | 21 |
| 3.1 | Superconducting circuits | 21 |
| 3.1.1 | Quantum and classical descriptions | 22 |
| 3.1.2 | LC resonator | 23 |
| 3.1.3 | Josephson junction | 24 |
| 3.1.4 | Cooper pair box | 25 |
| 3.2 | Transmon quantum computer model | 26 |
| 3.2.1 | Hamiltonian | 26 |
| 3.2.2 | Choice of the basis | 27 |
| 3.3 | Simulation toolkit | 31 |
| 3.3.1 | Numerical algorithm: <code>solver</code> | 32 |
| 3.3.2 | Evaluation of the results: <code>evaluator</code> | 38 |
| 3.3.3 | Visualization of the results: <code>visualizer</code> | 42 |
| 3.4 | Definition of the model systems | 42 |
| 3.4.1 | Single transmon-resonator system | 42 |
| 3.4.2 | Transmon-resonator system coupled to a bath | 42 |
| 3.4.3 | Two-transmon system | 44 |
| 3.4.4 | Small five-transmon system | 44 |
| 3.4.5 | Large five-transmon system | 44 |

| | | |
|----------|---|------------|
| 3.5 | Modeling electromagnetic environments | 48 |
| 3.5.1 | The Foster representation of an electromagnetic environment | 50 |
| 3.5.2 | Mapping to the model Hamiltonian | 52 |
| 4 | Free time evolution | 59 |
| 4.1 | Accuracy and performance benchmarks | 60 |
| 4.1.1 | Accuracy | 60 |
| 4.1.2 | Performance | 63 |
| 4.2 | Single transmon-resonator system | 68 |
| 4.2.1 | Overview of known perturbative results | 68 |
| 4.2.2 | Comparison to simulation results | 70 |
| 4.3 | Transmon-resonator system coupled to a bath | 72 |
| 4.3.1 | Simulation models | 73 |
| 4.3.2 | Results | 75 |
| 4.3.3 | Additional ways to improve the models | 79 |
| 4.4 | Effective ZZ interaction for coupled transmons | 80 |
| 4.5 | Conclusions | 83 |
| 5 | Optimizing pulses for quantum gates | 85 |
| 5.1 | Single-qubit pulses | 86 |
| 5.1.1 | The VZ gate | 87 |
| 5.1.2 | The GD pulse | 87 |
| 5.1.3 | The zero pulse | 88 |
| 5.2 | Two-qubit pulses | 89 |
| 5.2.1 | CNOT gates based on the CR effect | 89 |
| 5.2.2 | Analysis of IX and ZX interactions | 96 |
| 5.3 | Optimization of pulse parameters | 98 |
| 5.3.1 | The Nelder–Mead algorithm | 99 |
| 5.3.2 | Optimization results | 101 |
| 5.4 | Compiling quantum circuits | 105 |
| 5.5 | Alternative gate optimization techniques | 107 |
| 5.6 | Conclusions | 107 |
| 6 | Errors in quantum gates | 109 |
| 6.1 | Evaluation of gate metrics | 110 |
| 6.1.1 | Average gate fidelity | 110 |
| 6.1.2 | Diamond distance | 111 |
| 6.1.3 | Unitarity | 115 |
| 6.1.4 | Results | 116 |
| 6.2 | Repeated gate applications | 120 |
| 6.2.1 | Evolution of the diamond distance | 120 |
| 6.2.2 | Relation to experiments | 123 |
| 6.3 | Gate set tomography | 125 |
| 6.3.1 | The idea of GST | 126 |
| 6.3.2 | Running GST | 129 |

| | | |
|----------|---|------------|
| 6.3.3 | Predicting repeated pulse applications | 135 |
| 6.4 | Conclusions | 138 |
| 7 | Selected quantum circuit experiments | 141 |
| 7.1 | Crosstalk experiments | 142 |
| 7.1.1 | Circuit and simulation results | 142 |
| 7.1.2 | Comparison with experiments on the IBM Q Experience | 145 |
| 7.2 | Characterization of the singlet state | 147 |
| 7.2.1 | Experiment | 148 |
| 7.2.2 | Effective error model | 152 |
| 7.3 | Testing quantum fault tolerance | 155 |
| 7.3.1 | Fault-tolerant protocol | 156 |
| 7.3.2 | Test systems and circuits | 159 |
| 7.3.3 | Results | 161 |
| 7.4 | Conclusions | 165 |
| 8 | Discussion and conclusion | 167 |
| | Appendices | 171 |
| A | Visualization of quantum gate implementations | 173 |
| B | Elementary gate set used for the simulation | 176 |
| C | The reason for linear and unitary transformations in quantum theory | 178 |
| C.1 | Wigner's theorem | 178 |
| C.2 | Alternative approaches | 181 |
| C.3 | General remarks | 183 |
| D | Implementations of the four-component transformations V and V^\dagger | 184 |
| E | Error bounds for observables | 186 |
| F | Pulse parameters for quantum gates | 187 |
| G | Average fidelity of trace-decreasing quantum operations | 190 |
| G.1 | Preliminaries | 190 |
| G.2 | Quantum information theoretic proof | 191 |
| G.3 | Analytic proof | 192 |
| H | Diamond distance between unitary quantum operations | 194 |
| I | Proof of a diamond-distance bound for trace-decreasing operations | 196 |
| J | Gate decompositions and effective Hamiltonians | 198 |
| J.1 | The matrix logarithm | 199 |
| J.2 | Extracting the Hamiltonian | 199 |
| | Bibliography | 203 |
| | List of publications | 231 |
| | Eidesstattliche Erklärung | 233 |
| | Acknowledgments | 235 |

IAS Series
Band / Volume 45
ISBN 978-3-95806-505-5