



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).

Bibliography

- [1] D. Deutsch, *Quantum theory, the Church-Turing principle and the universal quantum computer*, Proceedings of the Royal Society of London A **400**, 97-117 (1985).
- [2] D. Deutsch, and R. Jozsa, *Rapid solution of problems by quantum computation*, Proceedings of the Royal Society of London A **439**, 553-558 (1992).
- [3] P. W. Shor, *Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer*, SIAM J. Comp. **26** (5), 1484-1509 (1997).
- [4] E. Bernstein, and U. Vazirani, *Quantum complexity theory*, SIAM Journal on Computing **26**, 1411-1473 (1997).
- [5] A. Montanaro, *Quantum algorithms: an overview*, npj Quantum Information **2**, 15023 (2016).
- [6] A. P. Lund, M. J. Bremner, and T. C. Ralph, *Quantum sampling problems, BosonSampling and quantum supremacy*, npj Quantum Information **3**, 15 (2017).
- [7] A. W. Harrow, and A. Montanaro, *Quantum computational supremacy*, Nature **549**, 203-209 (2017).
- [8] C. L. Degen, F. Reinhard and P. Cappellaro, *Quantum sensing*, Rev. Mod. Phys. **89**, 035002 (2017).
- [9] C. Zalka, *Shor's algorithm with fewer (pure) qubits*, ArXiv:quant-ph/0601097 (2013).
- [10] J. Smolin, G. Smith, and A. Vargo, *Oversimplifying quantum factoring*, Nature **499**, 163-165 (2013).
- [11] M. Born, *Zur Quantenmechanik der Stoßvorgänge*, Z. Physik **37**, 863-867 (1926).

Bibliography

- [12] L. E. Ballentine, *Quantum Mechanics: a modern development (2nd edition)*, (World Scientific Publishing Company (2014)).
- [13] M. Troyer, and U.-J. Wiese, *Computational Complexity and Fundamental Limitations to Fermionic Quantum Monte Carlo Simulations*, Phys. Rev. Lett. **94** (17), 170201 (2005).
- [14] G. Ortiz, J. Gubernatis, E. Knill, and R. Laflamme, *Quantum algorithms for fermionic simulations*, Phys. Rev. A **64**, 22319 (2001).
- [15] D. Poulin, M. B. Hastings, D. Wecker, N. Wiebe, A. C. Doherty, and M. Troyer, *The Trotter Step Size Required for Accurate Quantum Simulation of Quantum Chemistry*, Quantum Inf. and Comput. **15**, 361-384 (2015).
- [16] K. Sugisaki, S. Yamamoto, S. Nakazawa, K. Toyota, K. Sato, D. Shiomi, and T. Takui, *Quantum chemistry on quantum computers: a polynomial-time quantum algorithm for constructing the wave functions of open-shell molecules*, J. Phys. Chem. A **120**, 6459-6466 (2016).
- [17] F. Motzoi, M. P. Kaicher, and F. K. Wilhelm, *Linear and logarithmic time compositions of quantum many-body operators*, Phys. Rev. Lett. **119**, 160503 (2017).
- [18] Y. Cao, J. Romero, J. P. Olson, M. Degroote, P. D. Johnson, M. Kieferová, I. D. Kivlichan, T. Menke, B. Peropadre, N. P. D. Sawaya, S. Sim, L. Veis, and A. Aspuru-Guzik, *Quantum computational chemistry*, Chem. Rev. **119** (19), 10856-10915 (2019).
- [19] S. McArdle, S. Endo, A. Aspuru-Guzik, S. C. Benjamin, and X. Yuan, *Quantum chemistry in the age of quantum computing*, Rev. Mod. Phys. **92**, 015003 (2020).
- [20] M. M. Wilde, *Quantum Information and Entropy*, In *Quantum Information Theory (pp. 300-346)*, (Cambridge University Press (2017)).
- [21] W. J. Huggins, K. Wan, J. McClean, T. E. O'Brien, N. Wiebe, and R. Babbush, *Nearly optimal quantum algorithm for estimating multiple expectation values*, ArXiv:2111.09283 (2021).
- [22] N. Hansen, A. Auger, R. Ros, O. Mersmann, T. Tusar, and D. Brockhoff, *COCO: a platform for comparing continuous optimizers in a black-box setting*, Optim. Methods Softw. **36**, 114-144 (2021).

- [23] C. Doerr, F. Ye, N. Horesh, H. Wang, O. M. Shir, and T. Bäck, *Benchmarking discrete optimization heuristics with IOHprofiler*, Appl. Soft Comput. **88**, 106027 (2020).
- [24] T. Elsken, J. H. Metzen, and F. Hutter, *Neural Architecture Search: A Survey*, J. Mach. Learn. Res. **20**, 55:1-55:21 (2019).
- [25] H. Xiong, S. Shi, D. Ren, and J. Hu, *A survey of job shop scheduling problem: The types and models*, Comput. Oper. Res. **142**, 105731 (2022).
- [26] N. Khaneja, T. Reiss, C. Kehlet, T. Schulte-Herbrüggen, and S. J. Glaser, *Optimal control of coupled spin dynamics: design of NMR pulse sequences by gradient ascent algorithms*, Journal of Magnetic Resonance **172**, 296-305 (2005).
- [27] S. Machnes, U. Sander, S. J. Glaser, P. de Fouquières, A. Gruslys, S. Schirmer, and T. Schulte-Herbrüggen, *Comparing, optimizing, and benchmarking quantum-control algorithms in a unifying programming framework*, Phys. Rev. A **84**, 022305 (2011).
- [28] S. Machnes, E. Assémat, D. Tannor, and F. K. Wilhelm, *Tunable, Flexible, and Efficient Optimization of Control Pulses for Practical Qubits*, Phys. Rev. Lett. **120**, 150401 (2018).
- [29] F. Motzoi, *Controlling Quantum Information Devices*, PhD Thesis, U. Waterloo (2012).
- [30] M. A. Rol, *Control for programmable superconducting quantum systems*, PhD Thesis, TU Delft (2020).
- [31] J. D. Whitfield, J. Biamonte, and A. Aspuru-Guzik, *Simulation of electronic structure Hamiltonians using quantum computers*, Molecular Physics **109** (5), 735-750 (2011).
- [32] J. Hubbard, *Electron correlations in narrow energy bands*, Proceedings of the Royal Society of London A **276**, 1365 (1963).
- [33] J.P.F. LeBlanc, A. E. Antipov, F. Becca, I. W. Bulik, G. Kin-Lic Chan, C.-M. Chung, Y. Deng, M. Ferrero, T. M. Henderson, C. A. Jiménez-Hoyos, E. Kozik, X.-W. Liu, A. J. Millis, N. V. Prokof'ev, M. Qin, G. E. Scuseria, H. Shi, B.V. Svistunov, L. F. Tocchio, I.S. Tupitsyn, S. R. White, S. Zhang, B.-X. Zheng, Z. Zhu, and E. Gull, *Solutions of the two-Dimensional Hubbard model: benchmarks and*

Bibliography

- results from a wide range of numerical algorithms*, Phys. Rev. X **5**, 041041 (2015).
- [34] E. P. Wigner, and P. Jordan, *Über das Paulische Äquivalenzverbot*, Z. Phys. **47**, 631 (1928).
- [35] S. B. Bravyi, and A. Y Kitaev, *Fermionic quantum computation*, Ann. Phys. **298** (1), 210-266 (2002).
- [36] J. T. Seeley, M. J. Richard, and P. J. Love, *The Bravyi-Kitaev transformation for quantum computation of electronic structure*, J. Chem. Phys. **137** (22), 224109 (2012).
- [37] M. Steudtner, and S. Wehner, *Fermion-to-qubit mappings with varying resource requirements for quantum simulation*, New Journal of Physics **20** (6), 063010 (2018).
- [38] K. Setia, and J. D. Whitfield, *Bravyi-Kitaev Superfast simulation of electronic structure on a quantum computer*, J. Chem. Phys. **148**, 164104 (2018).
- [39] A. Peruzzo, J. McClean, P. Shadbolt, M-H. Yung, X-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'Brien, *A variational eigenvalue solver on a photonic quantum processor*, Nat. Comm. **5**, 4213 (2014).
- [40] M. Cerezo, A. Arrasmith, R. Babbush, S. C. Benjamin, S. Endo, K. Fujii, J. R. McClean, K. Mitarai, X. Yuan, L. Cincio, and P. J. Coles, *Variational quantum algorithms*, Nature Reviews Physics **3**, 625-644 (2021).
- [41] P. J. J. O'Malley, R. Babbush, I.D. Kivlichan, J. Romero, J. R. McClean, R. Barends, J. Kelly, P. Roushan, A. Tranter, N. Ding, B. Campbell, Y. Chen, Z. Chen, B. Chiaro, A. Dunsworth, A. G. Fowler, E. Jeffrey, E. Lucero, A. Megrant, J. Y. Mutus, M. Neeley, C. Neill, C. Quintana, D. Sank, A. Vainsencher, J. Wenner, T. C. White, P. V. Coveney, P. J. Lov, H. Neven, A. Aspuru-Guzik, and J. M. Martinis, *Scalable quantum simulation of molecular energies*, Phys. Rev. X **6**, 031007 (2016).
- [42] A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow, and J. M. Gambetta, *Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets*, Nature **549**, 242-246 (2017).

- [43] M. A. Nielsen, and I. L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press (2000).
- [44] R. Sagastizabal, X. Bonet-Monroig, M. Singh, M. A. Rol, C. C. Bultink, X. Fu, C. H. Price, V. P. Ostroukh, N. Muthusubramanian, A. Bruno, M. Beekman, N. Haider, T. E. O'Brien, and L. DiCarlo, *Experimental error mitigation via symmetry verification in a variational quantum eigensolver*, Phys. Rev. A **100**, 010302(R) (2019).
- [45] M. Ganzhorn, D.J. Egger, P. Barkoutsos, P. Ollitrault, G. Salis, N. Moll, M. Roth, A. Fuhrer, P. Mueller, S. Woerner, I. Tavernelli, and S. Filipp, *Gate-Efficient Simulation of Molecular Eigenstates on a Quantum Computer*, Phys. Rev. Applied **11**, 044092 (2019).
- [46] Google AI Quantum, and collaborators, *Hartree-Fock on a superconducting qubit quantum computer* Science **369** (6507), 1084-1089 (2020).
- [47] J. Preskill, *Quantum Computing in the NISQ era and beyond*, Quantum **2**, 79 (2018).
- [48] K. Bharti, A. Cervera-Lierta, T. Ha Kyaw, T. Haug, S. Alperin-Lea, A. Anand, M. Degroote, H. Heimonen, J. S. Kottmann, T. Menke, W-K. Mok, S. Sim, L-C. Kwek, and A. Aspuru-Guzik *Noisy intermediate-scale quantum algorithms*, Rev. Mod. Phys. **94**, 015004 (2022).
- [49] Y. Li, and S. C. Benjamin, *Efficient Variational Quantum Simulator Incorporating Active Error Minimization*, Phys. Rev. X **7**, 021050 (2017).
- [50] K. Temme, S. Bravyi, and J. M. Gambetta, *Error Mitigation for Short-Depth Quantum Circuits*, Phys. Rev. Lett. **119**, 180509 (2017).
- [51] S. Endo, S. C. Benjamin, and Y. Li, *Practical Quantum Error Mitigation for Near-Future Applications*, Phys. Rev. X **8**, 031027 (2018).
- [52] X. Bonet-Monroig, R. Sagastizabal, M. Singh, and T. E. O'Brien *Low-cost error mitigation by symmetry verification*, Phys. Rev. A **98**, 062339 (2018).
- [53] S. McArdle, X. Yuan, and S. C. Benjamin, *Error-Mitigated Digital Quantum Simulation*, Phys. Rev. Lett. **122**, 180501 (2019).

Bibliography

- [54] Z. Cai, *Quantum Error Mitigation using Symmetry Expansion*, *Quantum* **5**, 548 (2021).
- [55] W. J. Huggins, S. McArdle, T. E. O'Brien, J. Lee, N. C. Rubin, S. Boixo, K. Birgitta-Whaley, R. Babbush, and J. R. McClean, *Virtual Distillation for Quantum Error Mitigation*, *Phys. Rev. X* **11**, 041036 (2021).
- [56] B. Koczor, *Exponential Error Suppression for Near-Term Quantum Devices*, *Phys. Rev. X* **11**, 031057 (2021).
- [57] P. W. Shor, *Scheme for reducing decoherence in quantum computer memory*, *Phys. Rev. A* **52**, R2493 (1995).
- [58] A. M. Steane, *Error correcting codes in quantum theory*, *Phys. Rev. Lett.* **77**, 793 (1996).
- [59] D. Gottesman, *Class of quantum error-correcting codes saturating the quantum Hamming bound*, *Phys. Rev. A* **54**, 1862 (1996).
- [60] D. Gottesman, *Stabilizer Codes and Quantum Error Correction*, Ph.D. thesis, Caltech (1997).
- [61] S. B. Bravyi, and A. Y. Kitaev, *Quantum codes on a lattice with boundary*, ArXiv:quant-ph/9811052 (1998).
- [62] C. C. Bultink, T. E. O'Brien, R. Vollmer, N. Muthusubramanian, M. W. Beekman, M. A. Rol, X. Fu, B. Tarasinski, V. Ostroukh, B. Varbanov, A. Bruno, and L. DiCarlo, *Protecting quantum entanglement from leakage and qubit errors via repetitive parity measurements*, *Science Advances* **6** (12), eaay3050 (2020).
- [63] C. K. Andersen, A. Remm, S. Lazar, S. Krinner, N. Lacroix, G. J. Norris, M. Gabureac, C. Eichler, and A. Wallraff *Repeated quantum error detection in a surface code*, *Nat. Phys.* **16**, 875-880 (2020).
- [64] Y. Zhao, Y. Ye, H-L. Huang, Y. Zhang, D. Wu, H. Guan, Q. Zhu, Z. Wei, T. He, S. Cao, F. Chen, T-H. Chung, H. Deng, D. Fan, M. Gong, C. Guo, S. Guo, L. Han, N. Li, S. Li, Y. Li, F. Liang, J. Lin, H. Qian, H. Rong, H. Su, L. Sun, S. Wang, Y. Wu, Y. Xu, C. Ying, J. Yu, C. Zha, K. Zhang, Y-H. Huo, C-Y. Lu, C-Z. Peng, X. Zhu, and J-W. Pan, *Realization of an Error-Correcting Surface Code with Superconducting Qubits*, Arxiv:2112.13505 (2021).

- [65] H.-Y. Huang, R. Kueng, and J. Preskill, *Predicting many properties of a quantum system from very few measurements*, Nat. Phys. **16**, 1050-1057 (2020).
- [66] H.-Y. Huang, R. Kueng, and J. Preskill, *Efficient estimation of pauli Observables by derandomization*, Phys. Rev. Lett. **127**, (2021).
- [67] A. Zhao, N. C. Rubin, and A. Miyake, *Fermionic partial tomography via classical shadows*, Phys. Rev. Lett. **127**, (2021).
- [68] K. Wan, W. J. Huggins, J. Lee, and R. Babbush, *Matchgate shadows for fermionic quantum simulation*, ArXiv:2207.13723 (2021).
- [69] D. Ristè, S. Poletto, M.-Z. Huang, A. Bruno, V. Vesterinen, O.-P. Saira, and L. DiCarlo, *Detecting bit-flip errors in a logical qubit using stabilizer measurements*, Nat. Comm. **6**, 6983 (2015).
- [70] R. Barends, J. Kelly, A. Megrant, A. Veitia, D. Sank, E. Jeffrey, T. C. White, J. Mutus, A. G. Fowler, B. Campbell, Y. Chen, Z. Chen, B. Chiaro, A. Dunsworth, C. Neill, P. O'Malley, P. Roushan, A. Vainsencher, J. Wenner, A. N. Korotkov, A. N. Cleland, and J. M. Martinis, *Superconducting quantum circuits at the surface code threshold for fault tolerance*, Nature **508**, 441-445 (2014).
- [71] S. Debnath, N. M. Linke, C. Figgatt, K. A. Landsman, K. Wright, and C. Monroe, *Demonstration of a small programmable quantum computer with atomic qubits*, Nature **536**, 63-66 (2016).
- [72] T. Monz, D. Nigg, E. A. Martinez, M. F. Brandl, P. Schindler, R. Rines, S. X. Wang, I. L. Chuang, and R. Blatt, *Realization of a scalable Shor algorithm*, Science **351** (6277), 1068-1070 (2016).
- [73] N. Ofek, A. Petrenko, R. Heeres, P. Reinhold, Z. Leghtas, B. Vlastakis, Y. Liu, L. Frunzio, S. M. Girvin, L. Jiang, M. Mirrahimi, M. H. Devoret, and R. J. Schoelkopf, *Extending the lifetime of a quantum bit with error correction in superconducting circuits*, Nature **536**, 441 (2016).
- [74] N. Moll, P. Barkoutsos, L. S. Bishop, J. M. Chow, A. Cross, D. J. Egger, S. Filipp, A. Fuhrer, J. M. Gambetta, M. Ganzhorn, A. Kandala, A. Mezzacapo, P. Müller, W. Riess, G. Salis, J. Smolin, I. Tavernelli, and K. Temme, *Quantum optimization using variational algorithms on near-term quantum devices*, Quantum Science and Technology **3**, 3 (2018).

Bibliography

- [75] C. Neill, P. Roushan, K. Kechedzhi, S. Boixo, S. V. Isakov, V. Smelyanskiy, A. Megrant, B. Chiaro, A. Dunsworth, K. Arya, R. Barends, B. Burkett, Y. Chen, Z. Chen, A. Fowler, B. Foxen, M. Giustina, R. Graff, E. Jeffrey, T. Huang, J. Kelly, P. Klimov, E. Lucero, J. Mutus, M. Neeley, C. Quintana, D. Sank, A. Vainsencher, J. Wenner, T. C. White, H. Neven, and J. M. Martinis, *A blueprint for demonstrating quantum supremacy with superconducting qubits*, *Science* **360**, 195-199 (2018).
- [76] R. Babbush, N. Wiebe, J. McClean, J. McClain, H. Neven, and G. K-L. Chan, *Low-Depth Quantum Simulation of Materials*, *Phys. Rev. X* **8**, 011044 (2018).
- [77] D. Poulin, A. Kitaev, D. S. Steiger, M. B. Hastings, and M. Troyer, *Quantum Algorithm for Spectral Measurement with a Lower Gate Count*, *Phys. Rev. Lett.* **121**, 010501 (2018).
- [78] D. W. Berry, M. Kieferová, A. Scherer, Y. R. Sanders, G. H. Low, N. Wiebe, C. Gidney, and R. Babbush, *Improved techniques for preparing eigenstates of fermionic Hamiltonians*, *npj Quantum Information* **4**, 22 (2018).
- [79] I. D. Kivlichan, J. McClean, N. Wiebe, C. Gidney, A. Aspuru-Guzik, G. K-L. Chan, and R. Babbush, *Quantum Simulation of Electronic Structure with Linear Depth and Connectivity*, *Phys. Rev. Lett.* **120**, 110501 (2018).
- [80] A. Kandala, K. Temme, A. D. Corcoles, A. Mezzacapo, J. M. Chow, and J. M. Gambetta, *Error mitigation extends the computational reach of a noisy quantum processor*, *Nature* **567**, 491-495 (2019).
- [81] M. Otten, and S. K. Gray, *Recovering noise-free quantum observables*, *Phys. Rev. A* **99**, 012338 (2019).
- [82] J. R. McClean, M. E. Kimchi-Schwartz, J. Carter, and W. A. de Jong, *Hybrid quantum-classical hierarchy for mitigation of decoherence and determination of excited states*, *Phys. Rev. A* **95**, 042308 (2017).
- [83] J. I. Colless, V. V. Ramasesh, D. Dahlen, M. S. Blok, M. E. Kimchi-Schwartz, J. R. McClean, J. Carter, W. A. de Jong, and I. Siddiqi, *Computation of molecular spectra on a quantum processor with an error-resilient algorithm*, *Phys. Rev. X* **8**, 011021 (2018).

- [84] D. Gottesman, *An introduction to quantum error correction and fault-tolerant quantum computation*, Proc. Sympos. Appl. Math. **68**, 13 (2010).
- [85] B. M. Terhal, *Quantum error correction for quantum memories*, Rev. Mod. Phys. **87**, 307-346 (2015).
- [86] A. Y. Kitaev, *Quantum measurements and the Abelian Stabilizer Problem*, ArXiv:quant-ph/9511026 (1995).
- [87] J. R. McClean, J. Romero, R. Babbush, and A. Aspuru-Guzik, *The theory of variational hybrid quantum-classical algorithms*, New Journal of Physics **18**, 023023 (2016).
- [88] E. Farhi, J. Goldstone, and S. Gutmann, *A Quantum Approximate Optimization Algorithm*, ArXiv:1411.4028 (2014).
- [89] R. M. Parrish, L. A. Burns, D. G. A. Smith, A. C. Simmonett, A. E. DePrince, E. G. Hohenstein, U. Bozkaya, A. Y. Sokolov, R. Di Remigio, R. M. Richard, J. F. Gonthier, A. M. James, H. R. McAlexander, A. Kumar, M. Saitow, X. Wang, B. P. Pritchard, P. Verma, H. F. Schaefer, K. Patkowski, R. A. King, E. F. Valeev, F. A. Evangelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill *Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability*, Journal of Chemical Theory and Computation **13**, 3185-3197 (2017).
- [90] J. R. McClean, N. C. Rubin, K. J. Sung, I. D. Kivlichan, X. Bonet-Monroig, Y. Cao, C. Dai, E. S. Fried, C. Gidney, B. Gimby, P. Gokhale, T. Häner, Tarini Hardikar, V. Havlíček, O. Higgott, C. Huang, J. Izaac, Z. Jiang, X. Liu, S. McArdle, M. Neeley, T. O'Brien, B. O'Gorman, I. Ozfidan, M. D. Radin, J. Romero, N. P. D. Sawaya, B. Senjean, K. Setia, S. Sim, D. S. Steiger, M. Steudtner, Q. Sun, W. Sun, D. Wang, F. Zhang, and R. Babbush, *OpenFermion: the electronic structure package for quantum computers*, Quantum Science and Technology **5**, 034014 (2020).
- [91] D. Gottesman, *The Heisenberg Representation of Quantum Computers*, Group22: Proceedings of the XXII International Colloquium on Group Theoretical Methods in Physics, 32-43 (1999).
- [92] T. E. O'Brien, B. Tarasinski, and L. DiCarlo, *Density-matrix simulation of small surface codes under current and projected experimental noise*, npj Quantum Information **3**, 39 (2017).

Bibliography

- [93] S. Filipp, P. Maurer, P. J. Leek, M. Baur, R. Bianchetti, J. M. Fink, M. Göppl, L. Steffen, J. M. Gambetta, A. Blais, and A. Wallraff, *Two-Qubit state tomography using a joint dispersive readout*, Phys. Rev. Lett. **102**, 200402 (2009).
- [94] J. M. Chow, L. DiCarlo, J. M. Gambetta, A. Nunnenkamp, Lev S. Bishop, L. Frunzio, M. H. Devoret, S. M. Girvin, and R. J. Schoelkopf *Detecting highly entangled states with a joint qubit readout*, Phys. Rev. A **81**, 062325 (2010).
- [95] M. B. Hastings, D. Wecker, B. Bauer, and M. Troyer, *Improving quantum algorithms for quantum chemistry*, Quant. Inf. Comput. **15**, (2015).
- [96] I. M. Georgescu, S. Ashhab, and F. Nori, *Quantum simulation*, Rev. Mod. Phys. **86**, 153-185 (2014).
- [97] M. Suzuki, *Generalized Trotter's formula and systematic approximants of exponential operators and inner derivations with applications to many-body problems*, Comm. Math. Phys. **51**, 183-190 (1976).
- [98] C. Hempel, C. Maier, J. Romero, J. McClean, T. Monz, H. Shen, P. Jurcevic, B. P. Lanyon, P. Love, R. Babbush, A. Aspuru-Guzik, R. Blatt, and C. F. Roos, *Quantum chemistry calculations on a trapped-ion quantum simulator*, Phys. Rev. X **8**, 031022 (2018).
- [99] Y. Shen, X. Zhang, S. Zhang, J.-N. Zhang, M.-H. Yung, and K. Kim, *Quantum implementation of the unitary coupled cluster for simulating molecular electronic structure*, Phys. Rev. A **95**, 020501(R) (2017).
- [100] R. Santagati, J. Wang, A. Gentile, S. Paesani, N. Wiebe, J. McClean, S. Morley-Short, P. Shadbolt, D. Bonneau, J. Silverstone, D. Tew, X. Zhou, J. O'Brien, and M. Thompson, *Witnessing eigenstates for quantum simulation of Hamiltonian spectra*, Science Advances **4** (2018).
- [101] C. Kokail, C. Maier, R. van Bijnen, T. Brydges, M. Joshi, P. Jurcevic, C. Muschik, P. Silvi, R. Blatt, C. Roos, and P. Zoller, *Self-verifying variational quantum simulation of lattice models*, Nature **569**, 355-360 (2019).

- [102] M. Huo and Y. Li, *Self-consistent tomography of temporally correlated errors*, ArXiv:1811.02734 (2018).
- [103] J. McClean, S. Boixo, V. Smelyanskiy, R. Babbush, and H. Neven, *Barren plateaus in quantum neural network training landscapes*, Nature Communications **9**, 4812 (2018).
- [104] L. DiCarlo, J. M. Chow, J. M. Gambetta, L. S. Bishop, B. R. Johnson, D. I. Schuster, J. Majer, A. Blais, L. Frunzio, S. M. Girvin, and R. J. Schoelkopf, *Demonstration of two-qubit algorithms with a superconducting quantum processor*, Nature **460**, 240-244 (2009).
- [105] J. Majer, J. M. Chow, J. M. Gambetta, B. R. Johnson, J. A. Schreier, L. Frunzio, D. I. Schuster, A. A. Houck, A. Wallraff, A. Blais, M. H. Devoret, S. M. Girvin, and R. J. Schoelkopf, *Coupling superconducting qubits via a cavity bus*, Nature **449**, 443 (2007).
- [106] D. Brod and A. Childs, *The computational power of matchgates and the XY interaction on arbitrary graphs*, Quantum Information & Computation **14**, 901 (2014).
- [107] N. Hansen, *Benchmarking the Nelder-Mead downhill simplex algorithm with many local restarts*, in Proceedings of the 11th Annual Conference Companion on Genetic and Evolutionary Computation Conference: Late Breaking Papers, 2403-2408 (2009).
- [108] N. C. Rubin, R. Babbush, and J. McClean, *Application of fermionic marginal constraints to hybrid quantum algorithms*, New J. Phys **20**, 053020 (2018).
- [109] R. Blume-Kohout, *Optimal, reliable estimation of quantum states*, New J. Phys **12**, 043034 (2010).
- [110] Y.-K. Liu, M. Christandl, and F. Verstraete, *Quantum Computational Complexity of the N-Representability Problem: QMA Complete*, Phys. Rev. Lett. **98**, 110503 (2007).
- [111] O.-P. Saira, J. P. Groen, J. Cramer, M. Meretska, G. de Lange, and L. DiCarlo, *Entanglement Genesis by Ancilla-Based Parity Measurement in 2D Circuit QED*, Phys. Rev. Lett. **112**, 070502 (2014).
- [112] C. Dickel, J. J. Westdorp, N. K. Langford, S. Peiter, R. Sagastizabal, A. Bruno, B. Criger, F. Motzoi, and L. DiCarlo, *Chip-to-chip entanglement of transmon qubits using engineered measurement fields*, Phys. Rev. B **97**, 064508 (2018).

Bibliography

- [113] J. M. Chow, J. M. Gambetta, A. D. Córcoles, S. T. Merkel, J. A. Smolin, C. Rigetti, S. Poletto, G. A. Keefe, M. B. Rothwell, J. R. Rozen, M. B. Ketchen, and M. Steffen, *Universal Quantum Gate Set Approaching Fault-Tolerant Thresholds with Superconducting Qubits*, Phys. Rev. Lett. **109**, 060501 (2012).
- [114] D. Greenbaum, *Introduction to Quantum Gate Set Tomography*, ArXiv:1509.02921 (2015).
- [115] J. Romero, R. Babbush, J. R. McClean, C. Hempel, P. J. Love, and A. Aspuru-Guzik, *Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz*, Quantum Sci. Technol. **4**, 014008 (2018).
- [116] S. McArdle, A. Mayorov, X. Shan, S. Benjamin, and X. Yuan, *Quantum Computation of Molecular Vibrations*, Chem. Sci. **10**, 5725 (2019).
- [117] T. E. O'Brien, B. Senjean, R. Sagastizabal, X. Bonet-Monroig, A. Dutkiewicz, F. Buda, L. DiCarlo, and L. Visscher, *Calculating Energy Derivatives for Quantum Chemistry on a Quantum Computer*, npj Quantum Information **5**, 113 (2019).
- [118] Y. Nam, J-S. Chen, N. C. Pienti, K. Wright, C. Delaney, D. Maslov, K. R. Brown, S. Allen, J. M. Amini, J. Apisdorf, K. M. Beck, A. Blinov, V. Chaplin, M. Chmielewski, C. Collins, S. Debnath, K. M. Hudek, A. M. Ducore, M. Keesan, S. M. Kreikemeier, J. Mizrahi, P. Solomon, M. Williams, J. D. Wong-Campos, D. Moehring, C. Monroe, and J. Kim, *Ground-State Energy Estimation of the Water Molecule on a Trapped Ion Quantum Computer*, npj Quantum Information **6**, 33 (2019).
- [119] D. Wecker, M. B. Hastings, and M. Troyer, *Progress Towards Practical Quantum Variational Algorithms*, Phys. Rev. A **92**, 042303 (2015).
- [120] C. Overy, G. H. Booth, N. S. Blunt, J. J. Shepherd, D. Cleland, and A. Alavi, *Unbiased Reduced Density Matrices and Electronic Properties from Full Configuration Interaction Quantum Monte Carlo*, J. Chem. Phys. **141**, 244117 (2014).
- [121] G. Gidofalvi, and D. A. Mazziotti, *Molecular Properties from Variational Reduced-Density-Matrix Theory with Three-Particle N-representability Conditions*, J. Chem. Phys. **126**, 024105 (2007).

- [122] T. Takeshita, N. C. Rubin, Z. Jiang, E. Lee, R. Babbush, and J. R. McClean, *Increasing the Representation Accuracy of Quantum Simulations of Chemistry without Extra Quantum Resources*, Phys. Rev. X **10**, 011004 (2020).
- [123] J. Sethna, *Statistical Mechanics: Entropy, Order Parameters, and Complexity*, (Oxford University Press, New York, 2006).
- [124] J. Cotler, and F. Wilczek, *Quantum Overlapping Tomography*, Phys. Rev. Lett. **124**, 100401 (2020).
- [125] V. Verteletskyi, T.-C. Yen, and A. Izmaylov, *Measurement Optimization in the Variational Quantum Eigensolver Using a Minimum Clique Cover*, J. Chem. Phys. **152**, 124114 (2020).
- [126] R. M. Karp in *Complexity of Computer Computations*, edited by R. E. Miller, J. W. Thatcher, and J. D. Bohlinger (Springer, Boston, 1972).
- [127] A. Jena, S. Genin, and M. Mosca, *Pauli Partitioning with Respect to Gate Sets*, arXiv:1907.07859 (2019).
- [128] T.-C. Yen, V. Verteletskyi, and A. F. Izmaylov, *Measuring All Compatible Operators in One Series of a Single-Qubit Measurements Using Unitary Transformations*, J. Chem. Theory Comput. **16**, 4 (2020).
- [129] P. Gokhale, O. Angiuli, Y. Ding, K. Gui, T. Tomesh, M. Suchara, M. Martonosi, and F. T. Chong, *Minimizing State Preparations in Variational Quantum Eigensolver by Partitioning into Commuting Families*, arXiv:1907.13623 (2019).
- [130] A. F. Izmaylov, T.-C. Yen, R. A. Lang, and V. Verteletskyi, *Unitary Partitioning Approach to the Measurement Problem in the Variational Quantum Eigensolver Method*, J. Chem. Theory Comput. **16**, 1 (2020).
- [131] A. F. Izmaylov, T.-C. Yen, and I. G. Ryabinkin, *Revising Measurement Process in the Variational Quantum Eigensolver: Is It Possible to Reduce the Number of Separately Measured Operators?*, Chem. Sci. **10**, 3746 (2019).
- [132] W. J. Huggins, J. McClean, N. Rubin, Z. Jiang, N. Wiebe, B. Whaley, and R. Babbush, *Efficient and noise resilient measurements for*

Bibliography

- quantum chemistry on near-term quantum computers*, npj Quantum Information **7**, 23 (2021).
- [133] O. Crawford, B. van Straaten, D. Wang, T. Parks, E. Campbell, and S. Brierley, *Efficient quantum measurement of Pauli operators in the presence of finite sampling error*, Quantum **5**, 385 (2021).
- [134] A. Zhao, A. Tranter, W. M. Kirby, S. F. Ung, A. Miyake, and P. J. Love, *Measurement Reduction in Variational Quantum Algorithms*, Phys. Rev. A **101**, 062322 (2020).
- [135] A. N. Haberman, Carnegie Mellon University Technical Report No. AD-759-248, 1972.
- [136] F. Arute, K. Arya, R. Babbush, D. Bacon, J. C. Bardin, R. Barends, R. Biswas, S. Boixo, F. G. S. L. Brandao, D. A. Buell, and et al., *Quantum supremacy using a programmable superconducting processor*, Nature **574**, 505-510 (2019).
- [137] Q. Zhu, S. Cao, F. Chen, M.-C. Chen, X. Chen, T.-H. Chung, H. Deng, Y. Du, D. Fan, M. Gong, C. Guo, C. Guo, S. Guo, L. Han, L. Hong, H.-L. Huang, Y.-H. Huo, L. Li, N. Li, S. Li, Y. Li, F. Liang, C. Lin, J. Lin, H. Qian, D. Qiao, H. Rong, H. Su, L. Sun, L. Wang, S. Wang, D. Wu, Y. Wu, Y. Xu, K. Yan, W. Yang, Y. Yang, Y. Ye, J. Yin, C. Ying, J. Yu, C. Zha, C. Zhang, H. Zhang, K. Zhang, Y. Zhang, H. Zhao, Y. Zhao, L. Zhou, C.-Y. Lu, C.-Z. Peng, X. Zhu, and J.-W. Pan, *Quantum Computational Advantage via 60-Qubit 24-Cycle Random Circuit Sampling*, ArXiv:2109.03494 (2021).
- [138] K. M. Nakanishi, K. Fujii, and S. Todo, *Sequential minimal optimization for quantum-classical hybrid algorithms*, Phys. Rev. Research **2**, 043158 (2020).
- [139] M. Ostaszewski, E. Grant, and M. Benedetti, *Structure optimization for parameterized quantum circuits*, Quantum **5**, 391 (2021).
- [140] M. Wilson, R. Stromswold, F. Wudarski, S. Hadfield, N. M. Tubman, and E. G. Rieffel, *Optimizing quantum heuristics with meta-learning*, Quantum Machine Intelligence **3**, 13 (2021).
- [141] K. J. Sung, J. Yao, M. P. Harrigan, N. C. Rubin, Z. Jiang, L. Lin, R. Babbush, and J. R. McClean, *Using models to improve optimizers for variational quantum algorithms*, Quantum Science and Technology **5**, 044008 (2020).

- [142] X. Bonet-Monroig, R. Babbush and T. E. O'Brien, *Nearly optimal measurement scheduling for partial tomography of quantum state*, Phys. Rev. X **10**, 031064 (2020).
- [143] J. Wu, W. Hu, H. Xiong, J. Huan, V. Braverman, and Z. Zhu, *On the Noisy Gradient Descent that Generalizes as SGD*, 37th International Conference on Machine Learning, PMLR 119:10367-10376, (2020).
- [144] L. Yu, K. Balasubramanian, S. Volgushev, and M. A. Erdogdu, *An Analysis of Constant Step Size SGD in the Non-convex Regime: Asymptotic Normality and Bias*, CoRR (2020).
- [145] Z. Zhu, J. Wu, B. Yu, L. Wu, and J. Ma, *The Anisotropic Noise in Stochastic Gradient Descent: Its Behavior of Escaping from Sharp Minima and Regularization Effects*, *Proceedings of the 36th International Conference on Machine Learning, ICML 2019, 9-15 June 2019, Long Beach, California, USA*, Proceedings of Machine Learning Research **97**, 7654-7663 (2019).
- [146] C. Cade, L. Mineh, A. Montanaro, and S. Stanisic, *Strategies for solving the Fermi-Hubbard model on near-term quantum computers*, Phys. Rev. B **102**, 235122 (2020).
- [147] C. Doerr, F. Ye, N. Horesh, H. Wang, O. M. Shir, and T. Bäck, *Benchmarking discrete optimization heuristics with IOHprofiler*, App. Soft Computing **88**, 106027 (2020).
- [148] N. Hansen, D. Brockhoff, O. Mersmann, T. Tusar, D. Tusar, O. A. ElHara, P. R. Sampaio, A. Atamna, K. Varelas, U. Batu, D. M. Nguyen, F. Matzner, and A. Auger, *COMparing Continuous Optimizers: numbb/COCO on Github (v2.3)*, <https://doi.org/10.5281/zenodo.2594848>, Zenodo (2019)
- [149] M. López-Ibáñez, J. Dubois-Lacoste, L. Pérez Cáceres, M. Birattari, and T. Stützle, *The irace package: Iterated racing for automatic algorithm configuration*, Operations Research Perspectives **3**, 43-58 (2016).
- [150] J. C. Spall, *Multivariate stochastic approximation using a simultaneous perturbation gradient approximation*, IEEE Transactions on Automatic Control **37**, 332 (1992).
- [151] J. C. Spall, *John Hopkins apl technical digest* 19, 482 (1998).

Bibliography

- [152] M. J. D. Powell, *Direct search algorithms for optimization calculations*, Acta Numerica **7**, 287-336 (1998).
- [153] D. Kraft, *A software package for sequential quadratic programming*, Deutsche Forschungs- und Versuchsanstalt für Luft- und Raumfahrt Köln: Forschungsbericht (Wiss. Berichtswesen d. DFVLR, 1988).
- [154] D. Kraft, *Algorithm 733: TOMP-Fortran modules for optimal control calculations*, ACM Transactions on Mathematical Software **20**, 262-281 (1994).
- [155] *Sequential quadratic programming* in Numerical Optimization (Springer New York, New York, NY, 2006) pp. 529-562.
- [156] N. Hansen, and A. Ostermeier, *Completely Derandomized Self-Adaptation in Evolution Strategies*, Evolutionary Computation **9**, 159-195 (2001).
- [157] X. Bonet-Monroig, H. Wang, D. Vermetten, B. Senjean, C. Moussa, T. Back, V. Dunjko, and T. E. O'Brien, *Performance comparison of optimization methods on variational quantum algorithms (v0.1)*, <https://doi.org/10.5281/zenodo.5721349>, Zenodo (2021).
- [158] Cirq Developers, *Cirq 0.12.0*, <https://doi.org/10.5281/zenodo.5182845>, Zenodo (2021).
- [159] P. Virtanen, R. Gommers, T. E. Oliphant, M. Haberland, T. Reddy, D. Cournapeau, E. Burovski, P. Peterson, W. Weckesser, J. Bright, S. J. van der Walt, M. Brett, J. Wilson, K. J. Millman, N. Mayorov, A. R. J. Nelson, E. Jones, R. Kern, E. Larson, C. J. Carey, I. Polat, Y. Feng, E. W. Moore, J. VanderPlas, D. Laxalde, J. Perktold, R. Cimrman, I. Henriksen, E. A. Quintero, C. R. Harris, A. M. Archibald, A. H. Ribeiro, F. Pedregosa, P. van Mulbregt, and SciPy 1.0 Contributors, *SciPy 1.0: fundamental algorithms for scientific computing in Python*, Nature Methods **17**, 261-272 (2020).
- [160] N. Hansen, Y. Akimoto, and P. Baudis, *CMA-ES/pycma: r3.2.2*, <https://doi.org/10.5281/zenodo.2559634>, Zenodo (2019).
- [161] A. Mayer and S. O. Aas, *andim/noisyopt*, <https://doi.org/10.5281/zenodo.580120>, Zenodo (2017).
- [162] J. de Nobel, D. Vermetten, H. Wang, C. Doerr, and T. Bäck, *Tuning as a means of assessing the benefits of new ideas in interplay with*

- existing algorithmic modules*, in GECCO '21: Genetic and Evolutionary Computation Conference, Companion Volume, Lille, France, July 10-14, 2021 , edited by K. Krawiec (ACM) pp. 1375-1384 (2021).
- [163] D. Vermetten, H. Wang, T. Bäck, and C. Doerr, *Towards dynamic algorithm selection for numerical black-box optimization: investigating BBOB as a use case* in GECCO '20: Genetic and Evolutionary Computation Conference, Cancún Mexico, July 8-12, 2020 , edited by C. A. C. Coello (ACM) pp. 654-662 (2020).
- [164] I. W. Bulik, T. M. Henderson, and G. E. Scuseria, *Can single-reference coupled cluster theory describe static correlation?*, J. Chem. Theory Comput. **11**, 3171-3179 (2015).
- [165] R. J. Bartlett, and M. Musiał, *Coupled-cluster theory in quantum chemistry*, Rev. Mod. Phys. **79**, 291 (2007).
- [166] D. I. Lyakh, M. Musiał, V. F. Lotrich, and R. J. Bartlett, *Multireference nature of chemistry: The coupled-cluster view*, Chem. Rev. **112**, 182-243 (2012).
- [167] F. A. Evangelista, G. K.-L. Chan, and G. E. Scuseria, *Exact parameterization of fermionic wave functions via unitary coupled cluster theory*, J. Chem. Phys. **151**, 244112 (2019).
- [168] G. Greene-Diniz, and D. Muñoz Ramo, *Generalized unitary coupled cluster excitations for multireference molecular states optimized by the variational quantum eigensolver*, Int. J. Quantum Chem. **121**, e26352 (2021).
- [169] J. Lee, W. J. Huggins, M. Head-Gordon, and K. B. Whaley, *Generalized unitary coupled cluster wave functions for quantum computation*, J. Chem. Theory Comput. **15**, 311-324 (2018).
- [170] W. Mizukami, K. Mitarai, Y. O. Nakagawa, T. Yamamoto, T. Yan, and Y.-y. Ohnishi, *Orbital optimized unitary coupled cluster theory for quantum computer*, Phys. Rev. Research **2**, 033421 (2020).
- [171] I. O. Sokolov, P. K. Barkoutsos, P. J. Ollitrault, D. Greenberg, J. Rice, M. Pistoia, and I. Tavernelli, *Quantum orbital-optimized unitary coupled cluster methods in the strongly correlated regime: Can quantum algorithms outperform their classical equivalents?*, J. Chem. Theory Comput. **152**, 124107 (2020).

Bibliography

- [172] H. R. Grimsley, S. E. Economou, E. Barnes, and N. J. Mayhall, *An adaptive variational algorithm for exact molecular simulations on a quantum computer*, Nature Communications **10**, 1-9 (2019).
- [173] D. Claudino, J. Wright, A. J. McCaskey, and T. S. Humble, *Benchmarking adaptive variational quantum eigensolvers*, Frontiers in Chemistry **8**, 1152 (2020).
- [174] Y. S. Yordanov, V. Armaos, C. H. W. Barnes, and D. R. M. Arvidsson-Shukur, *Qubit-excitation-based adaptive variational quantum eigensolver*, Communications Physics **4**, 228 (2021).
- [175] N. Gomes, A. Mukherjee, F. Zhang, T. Iadecola, C.-Z. Wang, K.-M. Ho, P. P. Orth, and Y.-X. Yao, *Adaptive Variational Quantum Imaginary Time Evolution Approach for Ground State Preparation*, Advanced Quantum Technologies, 2100114 (2021).
- [176] J. Liu, Z. Li, and J. Yang, *An efficient adaptive variational quantum solver of the Schrödinger equation based on reduced density matrices*, J. Chem. Phys. **154**, 244112 (2021).
- [177] H. L. Tang, V. Shkolnikov, G. S. Barron, H. R. Grimsley, N. J. Mayhall, E. Barnes, and S. E. Economou, *qubit-ADAPT-VQE: An adaptive algorithm for constructing hardware-efficient ansätze on a quantum processor*, Phys. Rev. X Quantum **2**, 020310 (2021).
- [178] Z.-J. Zhang, T. H. Kyaw, J. Kottmann, M. Degroote, and A. Aspuru-Guzik, *Mutual information-assisted adaptive variational quantum eigensolver*, Quantum Science and Technology **6**, 035001 (2021).
- [179] H. R. Grimsley, D. Claudino, S. E. Economou, E. Barnes, and N. J. Mayhall, *Is the trotterized uccsd ansatz chemically well-defined?*, J. Chem. Theory Comput. **16**, 1-6 (2019).
- [180] M.-A. Filip, and A. J. Thom, *The Best of Both Worlds: Optimizing Quantum Hardware Resources with Classical Stochastic Methods*, ArXiv:2108.10912 (2021).
- [181] QuTech and TNO, *Quantum Inspire Home*, <https://www.quantum-inspire.com> (2018).
- [182] T. Last, N. Smakharadze, P. Eendebak, R. Versluis, X. Xue, A. Sammak, D. Brousse, K. Loh, H. Polinder, G. Scappucci, M. Veldhorst,

- L. Vandersypen, K. Maturova, J. Veltin, and G. Albrecht, *Quantum Inspire - QuTech's platform for co-development and collaboration in quantum computing*, Proc. of SPIE **11324** (2020).
- [183] QuTech and TNO, *Quantum Inspire Starmon-5 fact sheet*, <https://qutech.nl/wp-content/uploads/2020/04/3.-Technical-Fact-Sheet-Quantum-Inspire-Starmon-5.pdf> (2020).
- [184] S. P. Jordan, *Fast Quantum Algorithm for Numerical Gradient Estimation*, Phys. Rev. Lett. **95**, 050501 (2005).
- [185] S. Lloyd, *Universal Quantum Simulators*, Science **273**, 1073-1078 (1996).
- [186] M. Reiher, N. Wiebe, K. M. Svore, D. Wecker, and M. Troyer, *Elucidating reaction mechanisms on quantum computers*, Proc. Natl. Acad. Sci. U.S.A. **114**, 7555 (2017).
- [187] D. S. Abrams, and S. Lloyd, *Simulation of Many-Body Fermi Systems on a Universal Quantum Computer*, Phys. Rev. Lett. **79**, 2586 (1997).
- [188] C. Zalka, *Simulating quantum systems on a quantum computer*, Proc. Royal Soc. Lond. A **454**, 313 (1998).
- [189] A. Aspuru-Guzik, A. D. Dutoi, P. J. Love, and M. Head-Gordon, *Simulated Quantum Computation of Molecular Energies*, Science **309**, 1704-1707 (2005).
- [190] R. M. Dreizler, and E. K. U. Gross, *Density Functional Theory: An Approach to the Quantum Many-Body Problem*, (Springer, Berlin, Heidelberg, 1990).
- [191] I. Shavitt, and R. J. Bartlett, *Many-body methods in chemistry and physics: MBPT and coupled-cluster theory*, (Cambridge university press, 2009).
- [192] G. H. Booth, A. J. Thom, and A. Alavi, *Fermion Monte Carlo without fixed nodes: A game of life, death, and annihilation in Slater determinant space*, J. Chem. Phys. **131**, 054106 (2009).
- [193] F. Jensen, *Introduction to computational chemistry*, 2nd ed. (John Wiley & Sons, 2007).

Bibliography

- [194] P. Norman, K. Ruud, and T. Saue, *Principles and Practices of Molecular Properties: Theory, Modeling and Simulations*, (John Wiley & Sons, 2018).
- [195] H. B. Schlegel, *Geometry optimization*, Wiley Interdiscip. Rev. Comput. Mol. Sci. **1**, 790 (2011).
- [196] D. Marx, and J. Hutter, *Ab Initio Molecular Dynamics: Basic Theory and Advance Methods*, (Cambridge University Press, 2009).
- [197] J. C. Tully, *Molecular dynamics with electronic transitions*, J. Chem. Phys. **93**, 1061 (1990).
- [198] J. Behler, *Perspective: Machine learning potentials for atomistic simulations*, J. Chem. Phys. **145**, 170901 (2016).
- [199] Z. Li, and W. Liu, *First-order nonadiabatic coupling matrix elements between excited states: A Lagrangian formulation at the CIS, RPA, TD-HF, and TD-DFT levels*, J. Chem. Phys. **141**, 014110 (2014).
- [200] B. F. Curchod, U. Rothlisberger, and I. Tavernelli, *Trajectory-Based Nonadiabatic Dynamics with Time-Dependent Density Functional Theory*, ChemPhysChem, **14**, 1314-1340 (2013).
- [201] S. Faraji, S. Matsika, and A. I. Krylov, *Calculations of non-adiabatic couplings within equation-of-motion coupled-cluster framework: Theory, implementation, and validation against multi-reference methods*, J. Chem. Phys. **148**, 044103 (2018).
- [202] A. Gilyen, S. Arunachalam, and N. Wiebe, *Optimizing quantum optimization algorithms via faster quantum gradient computation*, Proceedings of the 2019 Annual ACM-SIAM Symposium on Discrete Algorithms (SODA), 1425-1444 (2019).
- [203] P.-L. Dallaire-Demers, J. Romero, L. Veis, S. Sim, and A. Aspuru-Guzik, *Low-depth circuit ansatz for preparing correlated fermionic states on a quantum computer*, Quantum Sci. Technol. **4**, 045005 (2019).
- [204] M. Schuld, V. Bergholm, C. Gogolin, J. Izaac, and N. Killoran, *Evaluating analytic gradients on quantum hardware*, Phys. Rev. A **99**, 032331 (2019).

- [205] A. Harrow, and J. Napp, *Low-Depth Gradient Measurements Can Improve Convergence in Variational Hybrid Quantum-Classical Algorithms*, Phys. Rev. Lett. **126**, 140502 (2021).
- [206] G. G. Guerreschi, and M. Smelyanskiy, *Practical optimization for hybrid quantum-classical algorithms*, ArXiv:1701.01450, (2017).
- [207] I. Kassal, and A. Aspuru-Guzik, *Quantum algorithm for molecular properties and geometry optimization*, J. Chem. Phys. **131**, 224102 (2009).
- [208] A. Roggero, and J. Carlson, *Dynamic linear response quantum algorithm*, Phys. Rev. C **100**, 034610 (2019).
- [209] L. Visscher, *The Dirac equation in quantum chemistry: Strategies to overcome the current computational problems*, J. Comp. Chem. **23**, 759 (2002).
- [210] E. Knill, G. Ortiz, and R. D. Somma, *Optimal quantum measurements of expectation values of observables*, Phys. Rev. A **75**, 012328 (2007).
- [211] D. Wecker, M. B. Hastings, N. Wiebe, B. K. Clark, C. Nayak, and M. Troyer, *Solving strongly correlated electron models on a quantum computer*, Phys. Rev. A **92**, 062318 (2015).
- [212] P.-L. Dallaire-Demers, and F. K. Wilhelm, *Method to efficiently simulate the thermodynamic properties of the Fermi-Hubbard model on a quantum computer*, Phys. Rev. A **93**, 032303 (2016).
- [213] B. Bauer, D. Wecker, A. J. Millis, M. B. Hastings, and M. Troyer, *Hybrid Quantum-Classical Approach to Correlated Materials*, Phys. Rev. X **6**, 031045 (2016).
- [214] R. M. Parrish, E. G. Hohenstein, P. L. McMahon, and T. J. Martinez, *Quantum Computation of Electronic Transitions Using a Variational Quantum Eigensolver*, Phys. Rev. Lett. **112**, 230401 (2019).
- [215] O. Higgott, D. Wang, and S. Brierley, *Variational Quantum Computation of Excited States*, Quantum **3**, 156 (2019).
- [216] T. Jones, S. Endo, S. McArdle, X. Yuan, and S. C. Benjamin, *Variational quantum algorithms for discovering Hamiltonian spectra*, Phys. Rev. A **99**, 062304 (2019).

Bibliography

- [217] R. J. Bartlett, *Coupled-cluster theory and its equation-of-motion extensions*, Wiley Interdiscip. Rev.: Comput. Mol. Sci. **2**, 126 (2011).
- [218] I. Kassal, S. P. Jordan, P. J. Love, M. Mohseni, and A. Aspuru-Guzik, *Polynomial-time quantum algorithm for the simulation of chemical dynamics*, Proc. Natl. Acad. Sci. U.S.A., 18681 (2008).
- [219] T. Saue, L. Visscher, H. J. Aa. Jensen, and R. Bast, with contributions from V. Bakken, K. G. Dyall, S. Dubillard, U. Ekström, E. Eliav, T. Enevoldsen, E. Faßhauer, T. Fleig, O. Fossgaard, A. S. P. Gomes, E. D. Hedegård, T. Helgaker, J. Henriksson, M. Iliaš, Ch. R. Jacob, S. Knecht, S. Komorovský, O. Kullie, J. K. Lærdahl, C. V. Larsen, Y. S. Lee, H. S. Nataraj, M. K. Nayak, P. Norman, G. Olejniczak, J. Olsen, J. M. H. Olsen, Y. C. Park, J. K. Pedersen, M. Pernpointner, R. di Remigio, K. Ruud, P. Sałek, B. Schimmelpennig, A. Shee, J. Sikkema, A. J. Thorvaldsen, J. Thyssen, J. van Stralen, S. Villaume, O. Visser, T. Winther, and S. Yamamoto, *DIRAC18 (v18.0)*, <https://doi.org/10.5281/zenodo.2253986>, Zenodo (2018).
- [220] B. Senjean, *Openfermion-Dirac*, (2022)
- [221] X. Fu, L. Rieseboos, M. A. Rol, J. van Straten, J. van Someren, N. Khammassi, I. Ashraf, R. F. L. Vermeulen, V. Newsum, K. K. L. Loh, J. C. de Sterke, W. J. Vlothuizen, R. N. Schouten, C. G. Almudever, L. DiCarlo, and K. Bertels, *eQASM: An Executable Quantum Instruction Set Architecture*, Proceedings of the 25th International Symposium on High-Performance Computer Architecture (HPCA'19), (2019).
- [222] A. Johnson, G. Ungaretti, and *et al.*, *QCoDeS*, (2016).
- [223] M.A. Rol, C. Dickel, S.Asaad, N.K. Langford, C.C. Bultink, R. Sagastizabal, N.K. Langford, G. de Lange, X. Fu, S.R. de Jong, F. Luthi, and W. Vlothuizen, *PycQED*, <https://doi.org/10.5281/zenodo.160327>, Zenodo (2016).
- [224] J. Nelder, and R. Mead, *A Simplex Method for Function Minimization*, Comp. J. **7**, (308) (1965).
- [225] T. H. Fischer, and J. Almöf, *General methods for geometry and wave function optimization*, J. Phys. Chem. **96**, 9768-9774 (1992).

- [226] Y. Yamaguchi, Y. Osamura, J. D. Goddard, and H. F. Schaefer III, *A New Dimension to Quantum Chemistry: Analytic Derivative Methods in Ab Initio Molecular Electronic Structure Theory*, (Oxford University Press: New York, Oxford, 1994).

