Biographical Sketch

James Daniel Whitfield

Contact

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Academic Appointments

06/2016 - Present **Assistant Professor of Physics**, Dartmouth College
Department of Physics and Astronomy

Postdoctoral Fellowships

2015-2016 **Postdoctoral Fellow**, University of Ghent (Ghent, Belgium)
Advisor: Frank Verstraete

2012-2015 **VCQ Postdoctoral Fellow**, Vienna Center for Quantum Science and Technology (Vienna, Austria)
Advisor: Frank Verstraete

2011-2012 **Postdoctoral Fellow**, Columbia University (New York, NY)
Advisors: Boris Altshuler

2011-2012 **Postdoctoral Fellow**, NEC Laboratories America (Princeton, NJ)
Advisors: Jérémie Roland

Education

2011 **Ph.D. Chemical Physics**, Harvard University (Cambridge, MA)
Thesis: *At the Intersection of Quantum Computing and Quantum Chemistry*
Advisor: Alán Aspuru-Guzik

2009 **A.M. Chemistry**, Harvard University (Cambridge, MA)

2006 **B.S. Mathematics and Chemistry**, *Magma cum laude*, Morehouse College (Atlanta, GA)

Awards

2016 Walter and Constance Berke Fellowship

2015 Ford Postdoctoral Fellowship

2011 Molecular Physics Young Author Prize, *Journal of Molecular Physics*
For "Simulation of electronic structure Hamiltonians using quantum computers"

2006-11 Harvard University Graduate Prize Fellowship, Harvard University

Professional Activities

2019 Achieving a Quantum Smart Workforce — Kavli Futures Symposium, Los Angeles, CA
2018 Participant, Summit on Advancing American Leadership in Quantum Information Science, White House
2018 Long-term visitor at Simons Institute; Workshop "Challenges in Quantum Computing" (UC Berkeley)
2018 NSF Young Investigator's Workshop
2017 American Association of Physics Teachers New Faculty Workshop participation
2017 Programme Committee for conference *Theory of Quantum Computation, Communication, and Cryptography*
2017 Ford Foundation Fellowships Review Panel
2015 Co-organized conference *Novel Computing Approaches to Quantum Chemistry*, Telluride, CO
2012 Visiting Scholar, Max Planck Institute for the Physics of Complex Systems, Condensed Matter Group
2012 Visiting Scientist, Institute for Scientific Interchange, Quantum Science Laboratory

Reviewer for various journals (Quantum Information and Computation, New Journal of Physics, Nature, Nature Communications, Physical Review A, Physical Review Letters, Quantum Science and Technology, Journal of Physics A: Mathematical and Theoretical, International Journal of Quantum Chemistry, NSF Ad-Hoc panels, Alexander von Humboldt Fellowship reviewer)

Professional memberships

- American Physical Society
- American Chemical Society

College Committees

- William H. Neukom Academic Cluster in Computational Science, Faculty search committee, Fall 2018 - Spring 2019
- Colloquium Committee member, Fall 2018 - Fall 2019
- Digital Outreach Committee chair, since Fall 2016
- Graduate Admissions and Policy committee member, since Fall 2016

Teaching

Fall 2016	Introduction to Condensed Matter, Phys 73
Spring 2017	Quantum Physics of Matter, Phys 40
Fall 2017	Introduction to Condensed Matter, Phys 73
Winter 2018	Introductory Physics I, Phys 13
Spring 2018	Quantum Information, Phys 116
Fall 2018	Introduction to Condensed Matter, Phys 73
Winter 2019	Introductory Physics I, Phys 13
Spring 2019	Quantum Physics of Matter, Phys 40

Undergraduate theses supervised

- Shaket Chaudhary, Undergraduate thesis 2019
  "Constructing Random Ensembles of Fermionic Systems"

- Erik Weis, Undergraduate thesis 2018
  "Benchmarking Quantum Computers Using Electronic Structure Algorithms"
- Samuel Greydanus, Undergraduate thesis 2017
  "Approximating Matrix Product States with Machine Learning"

Talks since 2016

Conference Presentations

- Theoretical Physics Symposium 2019 (invited speaker) — DESY Hamburg, Germany — November 2019
  - Quantum technology and time-dependent density functional theory — November 15, 2019
- Quantum Information for Developers Summer School and Hackathon (invited lecturer) — Swiss Federal Institute of Technology in Zürich (ETHZ) Zürich, Switerland — Sept 2019
  - Hamiltonian simulation problems and quantum chemistry — September 8, 2019
  - Fermions, bosons, and qubits — September 8, 2019
  - Time evolution and measurements of Hamiltonians — September 9, 2019
- Quantum Indeterminacy Workshop (invited talk) — Hanover, NH — July 2019
  - Computation versus Experiment: Quantum technology meets quantum computing — July 13, 2019
- American Mathematics Society Joint Mathematics Meeting (contributed talk) — Baltimore, MD — January 2019
  - Quantum Measurement Problem. Session: AMS Special Session on 25 years of Conferences for African-American Researchers in the Mathematical Sciences (CAARMS times 25), II. January 16, 2019
- American Physical Society Meeting (contributed talk) — Boston, MA — March 2019
  - Quantum simulation and Time-Dependent Density Functional Theory. Session: Applications of Noisy Intermediate Scale Quantum Computers III. March 5, 2019
- International Workshop on Quantum Chemical Calculations on Quantum Computers (invited talk) — Osaka City University (OCU), Osaka, Japan — March 2018
  - Fermionic Algebras for Quantum Computing. March 29, 2018

Invited Seminars/Colloquia

- Harvard University — Institute for Theoretical Atomic Molecular and Optical Physics — Cambridge, MA. Quantum Computing and Non-interacting Electronic Theories. November 7, 2019
- Naval Research Laboratory (Chemistry Colloquium) — Washington, D.C. Chemistry in the age of Quantum Supremacy. October 17, 2019
- Stony Brook University — Stony Brook, NY. Quantum Simulation of Fermions: Fermion-to-spin mappings and TDDFT. May 16, 2019
- Bates College — Lewiston, ME. The Promise of Quantum Technology. November 15, 2018
- Virginia Institute of Technology — Blacksburg, VA. Quantum Simulation of Fermions. Sept 10, 2018
- Microsoft — Redmond, Washington. Quantum Simulation and Applications. August 9, 2018

- Pacific Northwest Laboratories — Richland, Washington. Quantum Simulation of Fermions. August 7, 2018
- Rigetti Quantum Computing — Berkeley, CA. Hydrogen Quantum Simulation. July 18, 2018
- Simons Institute — Berkeley, CA. Formalizing Electronic Structure Problems. July 12, 2018
- Sandia National Laboratories — Livermore, California. Quantum Simulation of Fermions. July 9, 2018
- IBM T. J. Watson — Yorktown Heights, NY. Fermionic simulation on quantum computers, June 9, 2018
- Quantum Lunch Seminar at Los Alamos National Laboratory — Los Alamos, NM. Fermionic algebras for qubits, January 26, 2017
- Georgia Tech Quantum Information Seminar at Georgia Institute of Technology — Atlanta, GA. Electronic structure on quantum computers with ultra-local qubit operators. January 31, 2017

Funding since 2016

1. National Science Foundation, 2019-2023
   "EPSCoR RII Track-2 FEC: Harnessing the Data Revolution for the Quantum Leap: From Quantum Control to Quantum Materials," Co-I, $1,949k / 4 years.
2. Department of Energy Grant, 2019-2024
   "Fundamental Algorithmic Research for Quantum Computing," PI, $1,246k /5 years.
3. National Science Foundation Grant PHYS-1820747, 2018-2021
   "Topological Fermionic Quantum Simulation," PI, $407k /3 years.
4. Department of Energy Grant DE-SC0019374, 2018-2021
   "Quantum Chemistry for Quantum Computers," Co-PI, $536k/3 years.
5. Department of Energy Grant DE-SC0019374, 2018-2022
   "Optimization, Verification, and Engineered Reliability of Quantum Computers," Co-PI, $727k/4 years.

Papers since 2016

Citations reported from Google Scholar (h-index: 17, i10-index: 19)

1. K Setia, R Chen, J E Rice, A Mezzacapo, M Pistoia, James Daniel Whitfield. Reducing qubit requirements for quantum simulation using molecular point group symmetries. (Preprint) arXiv:1910.14644.
2. J Yang and J Brown and James Daniel Whitfield. Measurement on quantum devices with applications to time-dependent density functional theory. (Preprint) arXiv:1909.03078.
3. K Setia, S Bravyi, A Mezzacapo, James Daniel Whitfield. Superfast encodings for fermionic quantum simulation. Physical Review Research, 1, 033033, 2019.
4. R W Chien, S Xue, T S Hardikar, K Setia, James Daniel Whitfield. Analysis of Superfast Encoding Performance for Electronic Structure Simulations. Physical Review A, 100, 032337, 2019.
5. S Gulania, James Daniel Whitfield. Young frames for quantum chemistry. (Preprint) arXiv:1904.10469.
6. J Brown, J Yang, James Daniel Whitfield. Solver for the electronic V-representation problem of time-dependent density functional theory. (Preprint) arXiv:1904.10958.
7. J Brown, James Daniel Whitfield. Basis set convergence of Wilson basis functions for electronic structure. Journal of Chemical Physics, 151, 064118, 2019.

8. K Setia, James Daniel Whitfield. Bravyi-Kitaev Superfast simulation of fermions on a quantum computer. The Journal of Chemical Physics, 148, 164104, 2018.

9. C Schilling, M Altunbulak, S Knecht, A Lopes, James Daniel Whitfield, M Christandl, D Gross, M Reiher. Generalized Pauli constraints in small atoms. Physical Review A, 97, 052503, 2018.

10. G Zhu, Y Subasi, James Daniel Whitfield, M Hafezi. Hardware-efficient fermionic simulation with a cavity-QED system. New Physics Journal Quantum Information, 4, 16, 2018.

11. V Havlíček, M Troyer, James Daniel Whitfield. Operator Locality in Quantum Simulation of Fermionic Models. Physical Review A, 95, 032332, 2017.

12. James Daniel Whitfield, V Havlíček, M Troyer. Local spin operators for fermion simulations. Physical Review A, 94, 030301, 2016.

Other Publications

12. S Barz, B Dakic, Y O Lipp, F Verstraete, James Daniel Whitfield, P Walther. Linear-optical generation of eigenstates of the two-site XY model. Physical Review X, 5(2):021010, 2015.

13. Y Wang, F Dolde, J Biamonte, R Babbush, V Bergholm, S Yang, I Jakobi, P Neumann, A Aspuru-Guzik, James Daniel Whitfield, and J Wrachtrup. Quantum Simulation of Helium Hydride Cation in a Solid-State Spin Register. ACS Nano, 9(8):7769-7774, 2015.

14. James Daniel Whitfield, M-H Yung, D G Tempel, S Boixo, A Aspuru-Guzik. Computational complexity of time-dependent density functional theory. New Journal of Physics, 16(8):083035, 2014.

15. James Daniel Whitfield, Z Zimborás. On the NP-completeness of the Hartree-Fock method for translationally invariant systems. The Journal of Chemical Physics, 141(23):234103, 2014.

16. James Daniel Whitfield. Communication: Spin-free quantum computational simulations and symmetry adapted states. The Journal of Chemical Physics, 139:021105, 2013.

17. James Daniel Whitfield, P J Love, and A Aspuru-Guzik. Computational complexity in electronic structure. Physical Chemistry Chemical Physics, 15(2):397-411, 2013.

18. Z Zimboras, M Faccin, Z Kadar, James Daniel Whitfield, B Lanyon, and J Biamonte. Quantum transport enhancement by time-reversal symmetry breaking. Scientific Reports, 3:2361, 2013.

19. James Daniel Whitfield, M Faccin, and J D Biamonte. Ground-state spin logic. EPL (Europhysics Letters), 99(5):57004, 2012.

20. James Daniel Whitfield. Chapter 7 - Electronic Structure in "Mathematical Modeling II: Quantum Mechanics and Spectroscopy" by Troy L. Story. Zip Publishing, 2012.

21. N C Jones, James Daniel Whitfield, P L McMahon, M-H Yung, R Van Meter, A Aspuru-Guzik, and Y Yamamoto. Faster quantum chemistry simulation on fault-tolerant quantum computers. New Journal of Physics, 14(11):115023, 2012. (Citations: 92)

22. I Kassal, James Daniel Whitfield, A Perdomo-Ortiz, M-H Yung, and A Aspuru-Guzik. Simulating chemistry using quantum computers. Annual Review of Physical Chemistry, 62:185-207, 2011. (Citations: 211)

23. James Daniel Whitfield, J Biamonte, and A Aspuru-Guzik. Simulation of electronic structure Hamiltonians using quantum computers. Molecular Physics, 109(5):735-750, 2011. (Citations: 222)

24. J D Biamonte, V Bergholm, James Daniel Whitfield, J Fitzsimons, and A Aspuru-Guzik. Adiabatic quantum simulators. AIP Advances, 1(2):022126-022126, 2011.

25. Z Li, M-H Yung, H Chen, D Lu, James Daniel Whitfield, X Peng, A Aspuru-Guzik, and J Du. Solving quantum ground-state problems with nuclear magnetic resonance. Scientific Reports, 1, 2011.

26. B P Lanyon, James Daniel Whitfield, G G Gillett, M E Goggin, M P Almeida, I Kassal, J D Biamonte, M Mohseni, B J Powell, M Barbieri, et al. Towards quantum chemistry on a quantum computer. Nature Chemistry, 2(2):106-111, 2010. (Citations: 478)

27. M-H Yung, D Nagaj, James Daniel Whitfield, and A Aspuru-Guzik. Simulation of classical thermal states on a quantum computer: A transfer-matrix approach. Physical Review A, 82(6):060302, 2010.

28. James Daniel Whitfield, C A Rodriguez-Rosario, and A Aspuru-Guzik. Quantum stochastic walks: A generalization of classical random walks and quantum walks. Physical Review A, 81(2):022323, 2010. (Citations: 85)