Yuan Liu, Ph.D.

Assistant Professor
Department of Electrical and Computer Engineering
Department of Computer Science
Department of Physics (affiliated)
North Carolina State University

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EDUCATION

Ph.D., Chemical Physics 2015 – 2020
Department of Chemistry, Brown University

M.Sc., Electrical & Computer Engineering 2016 – 2018
School of Engineering, Brown University

B.S., Physics (with honors) 2011 – 2015
Department of Physics, Tsinghua University

RESEARCH INTERESTS

quantum algorithm and simulation, hybrid discrete-continuous variable quantum information processing, chemical physics, quantum engineering, quantum sensing, quantum signal processing

ACADEMIC APPOINTMENTS

Assistant Professor, NC State University, Raleigh NC 1/2024-present
Department of Electrical and Computer Engineering, Department of Computer Science

Adjunct Professor, NC State University, Raleigh NC 3/2024-present
Department of Physics

Adjunct Assistant Professor, NC State University, Raleigh NC 10/2023-12/2023
Department of Electrical and Computer Engineering

Postdoctoral Associate, Massachusetts Institute of Technology, Cambridge MA 07/2020-12/2023
Department of Physics, Research Laboratory of Electronics
Postdoc mentors: Professor Isaac L. Chuang, Professor Troy Van Voorhis

HONORS & AWARDS

- Postdoctoral Seed Funding Award (Co-PI), Co-Design Center for Quantum Advantage (C^2QA, National Quantum Information Science Research Center), U.S. Department of Energy, 2022 - 2023
- William R. Potter Prize for Doctoral Thesis of Outstanding Merit (1 per year, highest honor for graduate students in chemistry), Brown University, May 2020

- Chemical Computing Group Excellence Award, American Chemical Society National Meeting, Spring 2020
- Presidential Fellowship, Brown University, 2015 - 2018
- Sigma Xi Award, Brown University, 2019
- Open Graduate Education Fellowship and Travel award, Brown University, 2018 - 2020
- Conference Travel Grants, Chemistry Department, Brown University, 2017 - 2019
- Outstanding Undergraduate Thesis Award, Tsinghua University, 2015
- Top Prize, College Student Science and Technology Competition, Beijing, 2015
- Tsinghua Xue-Tang program and scholarship, Tsinghua University, 2013 - 2015

PUBLICATIONS

∗) Equal contribution
†) Corresponding author

Under review and in preparation

[U3] **Y. Liu***, S. Singh*, K. C. Smith*, and et al. *Hybrid Oscillator-Qubit Quantum Processors: Instruction Set Architectures, Abstract Machine Models, and Applications*. To be submitted to PRX Quantum.

[U2] Y. Liu et al. *Towards Mixed Analog-Digital Quantum Signal Processing: Quantum Digital-Analog Conversion and Quantum Fourier Transform.* To be submitted to IEEE Transactions on Signal Processing.

[U1] A. K. Tan†, **Y. Liu**†, C. M. Tran†, I. L. Chuang. *Error Correction of Quantum Algorithms: Arbitrarily Accurate Recovery Of Noisy Quantum Signal Processing*. Under review.

Peer-reviewed and published

[25] J. Sinanan-Sign*, G. L. Mintzer*, I. L. Chuang, **Y. Liu**† *Single-shot Quantum Signal Processing Interferometry*. Quantum (2024).

[24] J. Ang *et al. Architectures for Multinode Superconducting Quantum Computers*. To appear in ACM Transactions on Quantum Computing (2024).

[23] A. K. Tan†, **Y. Liu**†, C. M. Tran†, I. L. Chuang. *Perturbative Model of Noisy Quantum Signal Processing*. Phys. Rev. A **107**, 042429 (2023)

[22] **Y. Liu**†, O. Meitei, Z. E. Chin, A. Dutt, M. Tao, I. L. Chuang, T. Van Voorhis†. *Bootstrap Embedding on a Quantum Computer*. J. Chem. Theory Comput. **19**, 8, 2230–2247 (2023).

[21] D. F. Yuan, **Y. Liu**, Y. R. Zhang, L. S. Wang. *Observation of a Polarization-Assisted Dipole-Bound State*. J. Am. Chem. Soc. **145**, 9, 5512–5522 (2023).

[20] J. M. Martyn, **Y. Liu**, Z. E. Chin, I. L. Chuang. *Efficient Fully-Coherent Quantum Signal Processing Algorithms for Real-Time Dynamics Simulation*. J. Chem. Phys. **158** (2), 024106 (2023)

[19] B. Foulon, K. G. Ray, C. Kim, **Y. Liu**, V. Lordi, and B. M. Rubenstein. *1/ω Electric-field Noise in Surface Ion Traps from Correlated Adsorbate Dynamics*. Phys. Rev. A **105** (1), 013107 (2022).

[18] **Y. Liu**†, J. Sinanan-Singh, M. Kearney, G. Mintzer, I. Chuang. *Constructing Qudits from Infinite Dimensional Oscillators by Coupling to Qubits*. Phys. Rev. A **104**, 032605 (2021). **Editors' Suggestion**.

[17] D. F. Yuan, Y. R. Zhang, C. H. Qian, **Y. Liu**, L. S. Wang. *Probing the Dipole-Bound State in the 9-Phenanthrolate Anion by Photodetachment Spectroscopy, Resonant Two-Photon Photoelectron Imaging, and Resonant Photoelectron Spectroscopy*. J. Phys. Chem. A **125**, 14, 2967–2976 (2021).

[16] **Y. Liu**, G. Z. Zhu, D. F. Yuan, C. H. Qian, Y. R. Zhang, B. M. Rubenstein, and L. S. Wang. *Observation of a Symmetry-Forbidden Excited Quadrupole-Bound State*. J. Am. Chem. Soc. **142**, 47, 20240–20246 (2020).

[15] T. Shen, **Y. Liu**, Y. Yang, B. M. Rubenstein. *Finite Temperature Auxiliary Field Quantum Monte Carlo in the Canonical Ensemble*. J. Chem. Phys. **153**, 204108 (2020).

[14] D. F. Yuan*, **Y. Liu***, C. H. Qian, G. S. Kocheril, Y. R. Zhang, B. M. Rubenstein, and L. S. Wang. *Polarization of Valence Orbitals by the Intramolecular Electric Field From a Diffuse Dipole-Bound Electron*. J. Phys. Chem. Lett. **11**, 18, 7914–7919 (2020).

[13] D. F. Yuan*, **Y. Liu***, C. H. Qian, Y. R. Zhang, B. M. Rubenstein, and L. S. Wang. *Observation of a π-type Dipole-Bound State in Molecular Anions*. Phys. Rev. Lett. **125**, 073003 (2020).

[12] **Y. Liu**, T. Shen, H. Zhang, and B. M. Rubenstein. *Unveiling the Finite Temperature Physics of Hydrogen Chains via Auxiliary Field Quantum Monte Carlo*. J. Chem. Theory Comput. **16** 7, 4298–4314 (2020).

[11] B. L. Foulon, **Y. Liu**, J. K. Rosenstein, and B. M. Rubenstein. *A Language for Molecular Computation* (invited preview). Chem **5** (12), 3017 (2019).

[10] G. Z. Zhu, L. F. Cheung, **Y. Liu**, C. H. Qian, and L. S. Wang. *Resonant Two-Photon Photoelectron Imaging and Intersystem Crossing from Excited Dipole-Bound States of Cold Anions*. J. Phys. Chem. Lett. **10** (15), 4339 (2019).

[9] **Y. Liu**, C. G. Ning and L. S. Wang. *Double- and Multi-Slit Interference in Photodetachment from Nanometer Organic Molecular Anions*. J. Chem. Phys. **150** (24), 244302 (2019).

[8] **Y. Liu**, M. Cho, and B. M. Rubenstein. *Ab Initio Finite Temperature Auxiliary Field quantum Monte Carlo*. J. Chem. Theory Comput. **14**, 9, 4722 (2018).

[7] G. Z. Zhu, **Y. Liu**, Y. Hashikawa, Q. F. Zhang, Y. Murata, and L. S. Wang. *Probing the Interaction between the Encapsulated Water Molecule and the Fullerene Cages in $H_2O@C_{60}^-$ and $H_2O@C_{59}N^-$*. Chemical Science, **9**, 5666 (2018).

[6] G. Z. Zhu, Y. Hashikawa, **Y. Liu**, Q. F. Zhang, L. F. Cheung, Y. Murata, and L. S. Wang. *High-Resolution Photoelectron Imaging of Cryogenically-Cooled $C_{59}N^-$ and $(C_{59}N)_{22}^-$ Azafullerene Anions*. J. Phys. Chem. Lett. **8**, 6220 (2017).

[5] G. Z. Zhu, **Y. Liu** and L. S. Wang. *Observation of Excited Quadrupole-Bound States in Cold Anions*. Phys. Rev. Lett. **119**, 023002 (2017).

[4] D. L. Huang, G. Z. Zhu, **Y. Liu**, and L. S. Wang. *Photodetachment Spectroscopy and Resonant Photoelectron Imaging of Cryogenically-cooled Deprotonated 2-hydroxypyrimidine Anions*. J. Mol. Spectrosc. **332**, 86 (2017).

[3] **Y. Liu** and C. G. Ning. *Calculation of Photodetachment Cross Sections and Photoelectron Angular Distributions of Negative Ions Using Density Functional Theory*. J. Chem. Phys. **143**, 144310 (2015).

[2] H. T. Liu, D. L. Huang, **Y. Liu**, L. F. Cheung, P. D. Dau, C. G. Ning, and L. S. Wang. *Vibrational State-Selective Resonant Two-Photon Photoelectron Spectroscopy of AuS^- via a Spin-Forbidden Excited State*. J. Phys. Chem. Lett. **6**, 637 (2015).

[1] **Y. Liu**, L. F. Cheung and C. G. Ning. *Assessment of Delocalized and Localized Molecular Orbitals through Electron Momentum Spectroscopy*. Chin. Phys. B **23**, 063403 (2014). **Editors' Suggestion**.

THESIS

Ph.D. Thesis (Advisors: Brenda M. Rubenstein, Lai-Sheng Wang): *Finite Temperature Physics of Molecules and Solids via Auxiliary Field Quantum Monte Carlo and Observation of p-Type Dipole-Bound States Near the Molecular Threshold.*

B.S. Thesis (Advisor: Chuan-Gang Ning): *Calculation of Photoelectron Angular Distributions.*

CONFERENCE and SYMPOSIUM Presentations

- (Invited) 4th Annual Quantum Symposium at NC State University, "Toward Mixed Analog-Digital Quantum Signal Processing", Raleigh, NC, June 2024.
- American Conference on Theoretical Chemistry (ACTC), "Bootstrap embedding on a quantum computer", Chapel Hill, June 2024.
- (Invited) APS March Meeting, "Opportunities and challenges of bosonic oscillators for quantum computation and information processing", in the "From NISQ to Fault Tolerance" Symposium, March 2024, Minneapolis MN.
- (Theory Keynote) Co-Design Center for Quantum Advantage (C^2QA) All Hands Meeting, "Instruction Set Architecture and Abstract Machine Models for Hybrid Oscillator-Qubit Processors", Department of Energy, October 2023.
- Quantum Sensing Gordon Research Seminar, "Quantum Advantage in Continuous-Variable Algorithmic Sensing", Les Diablerets, VD, Switzerland, July 2023.
- (Invited) ACS Northeast Regional Meeting (NERM), "New quantum algorithms for old challenges: from real-time dynamics to electronic structure theory", Boston, June 2023.
- Flash talk at the Co-Design Center for Quantum Advantage (C^2QA) all hands meeting, "Bootstrap Embedding on a Quantum Computer", Yale University, October 2022.
- Conference on Quantum Information and Quantum Control IX (CQIQC-IX), "Constructing qudits from infinite-dimensional oscillators by coupling to qubits", September 2022, Toronto.
- American Chemical Society Fall Meeting, "Efficient-Fully Coherent Hamiltonian Simulation", August 2022, Chicago.
- American Chemical Society Fall Meeting, "Observation of a symmetry-forbidden excited quadrupole-bound state", August 2022, Chicago.
- IBM-MIT Quantum Information Theory Meeting, "Efficient-Fully Coherent Hamiltonian Simulation", March 2022, Massachusetts Institute of Technology, Cambridge MA.

- American Physical Society March Meeting, "Constructing Qudits from Infinite Dimensional Oscillators by Coupling to Qubits", March 2021, Virtual.
- MIT-NTT Quantum Information Group Meeting, "Constructing Qudits from Infinite Dimensional Oscillators by Coupling to Qubits", February 2021, Virtual.
- American Physical Society National Meeting, "Ab initio Finite Temperature Auxiliary Field Quantum Monte Carlo", March 2018, Los Angeles CA.

SEMINARS

- Condensed Matter Seminar, "Opportunities and challenges of bosonic oscillators for quantum computation and information processing", University of Tennessee at Knoxville, May 2024, Knoxville TN.
- Seminar, "New Quantum Algorithms for Old Challenges: From Quantum Simulation to Quantum Sensing", Oak Ridge National Laboratory, TN, April 2024.
- Quantum Information Seminar, "New Quantum Algorithms for Old Challenges: From Quantum Simulation to Quantum Error Correction", University of Cambridge, Cambridge UK, February 2024.
- CAMM & Condensed Matter Physics Seminar, "New Quantum Algorithms for Old Challenges: From Quantum Simulation to Quantum Error Correction", The University of Tennessee, Knoxville TN, November 2023.
- "New Quantum Algorithms for Old Challenges: From Quantum Simulation to Quantum Error Correction", Hong Kong University of Science and Technology, April 2023.
- Triangle Quantum Computing Seminar, "Error Correction of Quantum Algorithms: Arbitrarily Accurate Recovery of Noisy Quantum Signal Processing", Duke University, March 2023.
- "Toward efficient, scalable, and robust quantum algorithms for chemical physics", North Carolina State University, March 2023.
- Physics colloquium, "Towards efficient, scalable, and robust quantum algorithms for chemical physics", Virginia Tech, February 2023.
- Quantum Seminar at IBM Research, "Quantum Advantage of Embedding for Quantum Chemistry", Cambridge MA, February 2023.
- Seminar (virtual) at the InQubator for Quantum Simulation, "Efficient-Fully Coherent Quantum Signal Processing Algorithms for Real-Time Dynamics Simulation", University of Washington, November 2022.
- Talk at QuEra Computing Inc., "Bootstrap Embedding on a Quantum Computer", November 2022.
- Quanta Research Laboratory, "Double- and Multi-slit Interference of Photoelectrons from Organic Molecular Anions", Massachusetts Institute of Technology, February 2020, Cambridge MA.

TEACHING

- Instructor, Quantum Algorithms for Physical Sciences, NC State University, Spring 2024. *(Created a new graduate-level course on quantum algorithms and applications to physical science simulation in the Departments of Electrical & Computer Engineering and Computer Science.)*
- Kaufman Teaching Certificate Program, Massachusetts Institute of Technology, Fall 2021. *(A semester-long workshop on developing teaching skills systematically, with two micro-teaching demonstrations in a real classroom setting)*
- Teaching Assistant, Chemistry 1150 (Spring 2017) Physical Chemistry: Thermodynamics and Statistical Mechanics. Instructor: Prof. Lai-Sheng Wang. *(Responsible for holding office hours, creating problem sets, and grading homework)*

POSTDOCS & STUDENTS

Postdocs:

- Joel Bierman, postdoc, NC State – 2024 - present

Graduate students:

- Aishwarya Majumdar, PhD (Electrical & Computer Engineering), NC State – 2024-present
- Shariful Islam, PhD (Physics), NC State – 2024-present
- Elin Das, PhD (Electrical & Computer Engineering), NC State – 2024-present
- Daniel Dong, Masters (Computer Science) – 2024-present
- Manideepika Reddy Myaka, Masters (Computer Science), NC State – 2024-present

Visiting Students:

- Langxu Bai, Undergrad (Physics), Nankai University, 2024-present
- Leonard Li, Undergrad (Computer Science & Technology), Nanjing University, July 2024
- Lingjun Xiong, Undergrad (Physics), Huazhong University of Science and Technology (HUST), July 2024

Former Group Members:

- Nitin Joseph, Masters (Electrical & Computer Engineering), NC State – 2024
- Mihir Nikam, Masters (Computer Science), NC State – 2024

LEADERSHIP, SERVICE & OUTREACH

Reviewer

Programs: NSF: Mid-Scale Research Infrastructure, ENG/ECCS

Journals: *PRX Quantum, Quantum, Physical Review Letters, Physical Review A, Physical Review R, New Journal of Physics, Journal of Physical Chemistry, Journal of Chemical Theory and Computation, Chemical Physics.*

Conference Program Committee (PC)

- QCE24, PC member, Technical Paper Track on Quantum Applications, Poster Track, Montreal, Québec, Canada, September 2024.

NC State Electrical & Computer Engineering Department Thesis Committees – Member, January 2024 - Present

- Amey Meher (Zhou Group, Master 2024)
- Zachary Parks (Dreher Group, Ph.D. 2025 expected)

OTHER

- Session chair for "Quantum Computing for Tackling Challenges in Quantum Chemistry Symposium", ACS Fall Meeting, San Francisco, August 2023.
- Outreach lecture at Bexley high school (virtual, Ohio) on quantum science and technology via the Quantum To-Go project of American Physical Society, April 2023.
- Session chair for the quantum science and engineering center annual research conference (QuARC), Massachusetts Institute of Technology, February 2022.
- Judge (multiple times) for K-12 Science and Engineering Fairs: Massachusetts Science & Engineering Fair, Boston MA, April 2021; Times Squared Academy Science and Engineering Fair, Providence RI, February 2020; Rhode Island Science and Engineering Fair, Community College of Rhode Island, April 2016.
- Brown University Chemistry Department – Graduate student leadership committee, journal club co-organizer, September 2016 - May 2018.
- 4th Annual STEM Day of Brown University Chemistry Department, January 2020.