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

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

- 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
- Outstanding Undergraduate Thesis Award, Tsinghua University, 2015

- Top Prize, College Student Science and Technology Competition, Beijing, 2015
- Tsinghua Academic Talent Scholarship, Tsinghua University, 2013 - 2015

PUBLICATIONS

∗) Equal contribution
†) Corresponding author

Under review and in preparation

[U7] Victor M. Bastidas, Nathan Fitzpatrick, K. J. Joven, Zane M. Rossi, Shariful Islam, Troy Van Voorhis, Isaac L. Chuang, **Yuan Liu**†. *Unification of Finite Symmetries in Simulation of Many-body Systems on Quantum Computers*. Under review in PRX.

[U6] **Y. Liu***, Shraddha Singh*, Kevin C Smith*, Eleanor Crane, John M Martyn, Alec Eickbusch, Alexander Schuckert, Richard D Li, Jasmine Sinanan-Singh, Micheline B Soley, Takahiro Tsunoda, Isaac L Chuang, Nathan Wiebe, Steven M Girvin. *Hybrid Oscillator-Qubit Quantum Processors: Instruction Set Architectures, Abstract Machine Models, and Applications*. Under review in PRX.

[U5] John M Martyn, Zane M Rossi, Kevin Z Cheng, **Y. Liu**, Isaac L Chuang *Parallel Quantum Signal Processing Via Polynomial Factorization*. Under review in Quantum.

[U4] Xi Lu, **Y. Liu**, Hongwei Lin. *Quantum Signal Processing and Quantum Singular Value Transformation on $U(N)$*. Under review in Quantum.

[U3] A. K. Tan†, **Y. Liu**†, C. M. Tran†, I. L. Chuang. *Error Correction of Quantum Algorithms: Arbitrarily Accurate Recovery Of Noisy Quantum Signal Processing*. arXiv preprint.

[U2] **Y. Liu**†*, John M. Martyn*, Jasmine Sinanan-Singh, Kevin C. Smith, Steven M. Girvin, Isaac L. Chuang. *Toward Mixed Analog-Digital Quantum Signal Processing: Quantum AD/DA Conversion and the Fourier Transform*. Under review in IEEE Transactions on Signal Processing.

[U1] Nam Vu*, Daniel Dong*, Xiaohan Dan, Alec Eickbusch, Benjamin Brock, Ningyi Lyu,Di Luo, Victor Batista, **Y. Liu**†. *Co-Design Approach to Bosonic Hardware-Efficient Quantum Simulation of Dissipative Vibronic Dynamics*. In preparation for the Journal of Chemical Physics.

Journal Articles

[25] J. Sinanan-Sign*, G. L. Mintzer*, I. L. Chuang, **Y. Liu**†. *Single-shot Quantum Signal Processing Interferometry*. Quantum **8**, 1427 (2024). NC State News Press.

[24] J. Ang *et al.* *ARQUIN: Architectures for Multinode Superconducting Quantum Computers*. ACM Transactions on Quantum Computing **5**, 3 (19), 1-59 (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 $(C_{59}N)_{22}^-$ Aza-fullerene 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.

Conference Articles

[2] Amey Meher, **Y. Liu**, Huiyang Zhou. *Error Mitigation of Hamiltonian Simulations from an Analog-based Compiler (SimuQ)*. IEEE International Conference on Quantum Computing and Engineering (QCE), 2024.

[1] Tarini S. Hardikar, Kenneth Heitritter, James Brown, Ruhee D'Cunha, Abhishek Mitra, Shaun Weatherly, **Y. Liu**, Matthew Otten, Troy Van Voorhis, Laura Gagliardi, and Kanav Setia. *Quanta-Bind: A quantum computing pipeline for strongly correlated systems for Alzheimer's disease*. IEEE International Conference on Quantum Computing and Engineering (QCE), 2024.

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.*

SELECTED CONFERENCE and SYMPOSIUM Presentations

- (Tutorial) Organizer and presenter of APS March-April Meeting (Global Physics Summit) Tutorial on "Hybrid Continuous-Discrete Variable Quantum Computation", Anaheim CA, March 2025 (together with speakers from IBM, ETH Zurich, UMass Amherst).
- (Invited) Southeast Quantum Workshop, Talk on "Hybrid Oscillator-Qubit Quantum Processors: Instruction Set Architectures, Abstract Machine Models, and Applications", University of Tennessee, Knoxville, November 2024.
- QuantumOS Workshop (QuantumOS), Poster on "Protocols and Applications of Quantum Stack Memory", Austin TX, October 2024.
- Southwest Quantum Information and Technology Workshop (SQuInT), Talk on "Hybrid Oscillator-Qubit Quantum Processors: Instruction Set Architectures, Abstract Machine Mod-

els, and Applications", organized by the Center for Quantum Information and Control (CQuIC), Boulder CO, October 2024.

- (Invited) Workshop on Quantum Computation Beyond Gate-model, "Hybrid Oscillator-Qubit Quantum Processors: Instruction Set Architectures, Abstract Machine Models, and Applications", QuICS, University of Maryland, October 2024.
- (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.

SELECTED INVITED SEMINARS

- Colloquium, "Simulating Physical Sciences on Quantum Computers", Department of Physics, Virginia Commonwealth University, Richmond, VA.
- Seminar, "Opportunities and Challenges of Quantum Sensing for Health", ASSIST Center, North Carolina State University, October 2024

- Colloquium, "Quantum Signal Processing Interferometry: Pushing the Limit of Sensing with Quantum Algorithms", North Carolina State University, Department of Electrical and Computer Engineering, August 2024.
- 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 Ranjan Das, PhD (Electrical & Computer Engineering), NC State – 2024-present
- Daniel Dong, Masters (Computer Science) – 2024-present

Undergraduate Students:

- Loren Holl (Computer Science, 2025)
- Anthony Donelli (Computer Engineering, 2025)
- Rosalie Rutten (Computer Science, 2026)

Visiting Students:

- Langxu Bai, Undergrad (Physics), Nankai University, 2024-present
- Xi Lu, Ph.D. (Mathematics), Zhejiang University, 2024-present

Former Group Members:

- Manideepika Reddy Myaka, Masters (Computer Science), NC State – 2024
- Leonard Li, Undergrad (Computer Science & Technology), Nanjing University, July 2024
- Lingjun Xiong, Undergrad (Physics), Huazhong University of Science and Technology (HUST), July 2024
- 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, Reports on Progress in Physics, npj Quantum Information, Quantum Science and Technology, New Journal of Physics, Journal of Physical Chemistry, Journal of Chemical Theory and Computation, Chemical Physics.*

Conference Program Committee (PC) and Organizer

- Global Physics Summit (Joint APS March-Aprial Meeting), Organizer, Tutorial of Hybrid Continuious-Discrete Variable Quantum Computation, Anaheim, CA, 2025.
- 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.

GRANTS

1. *Achieving Quantum Utility with Hybrid Discrete Continuous Variable Quantum Processors*, Department of Energy, Office of Science Scientific Computing Research (ASCR). Principal Investigator, in collaboration with Rutgers University, UMass Amherst, NASA Ames, PNNL, and LBNL. 9/1/2024 - 8/31/2029. Total: $10.6M.
2. *Quanta-Bind: Demystifying Proteins*, sub-award from qBraid, Inc, Wellcome Leap Foundation, Quantum4Bio program. 2024/1 - 2025/3.
3. *Phase Space Formulation and Simulation of Molecular Conical Intersections*, RQS Seed Funding, University of Maryland (UMD). Principal Investigator, in collaboration with NIST and UMD. 9/1/2024 - 8/31/2025. Total: $80k.
4. *QACTI: Quantum Advantage-Class Trapped Ion Systems*, sub-award from Duke University, pilot project for National Quantum Virtual Laboratory (NVQL), National Science Foundation. 8/2024 - present