



Education



Purdue University,

PhD Candidate, Chemistry, Research Area: Quantum Computation,
Supervisor: Prof. Sabre Kais

2021–26,



Indian Institute of Technology, Kharagpur,

Integrated BSc. and MSc. Physics (Major). **8.91/10**,
Computer Science and Engineering (Minor)

2016–21,

Awards and Achievements

- **Ross Fellowship:** Awarded to Doctoral candidates at Purdue to recognize academic excellence. 2021
- **INSPIRE Scholarship:** Awarded by the Govt. of India to high-achieving students in sciences. 2016-21
- **Future Research Talent Travel Award:** A program for exceptional international students to pursue collaborative research in Sciences at the Australian National University. 2019

Publications/Presentations

- **Application of machine learning to two-dimensional Dzyaloshinskii-Moriya ferromagnets**, V.K. Singh and J.H. Han, PhysRevB.99.174426. 2019
- **Quantum Neural Networks for Analysing X-Ray Scattering Data**, V.K. Singh and Brenda Rubenstein, IEEE QCE20 Poster. 2020
- **Statistical recovery of the classical spin Hamiltonian**, V.K. Singh and J.H. Han, arXiv:1807.04884. 2018

Research Experience



University of California, Berkeley,

Electrical Engineering and Computer Science,

Supervisors: Prof. Umesh Vazirani and Prof. Zeph Landau,

May 2021-Present

Tensor Networks and AGSP.

- Implemented GPU-accelerated Tensor Network Architecture by combining MPNUM and CuPy.
- Studied the evolution of a quantum state under the action of an Approximate Ground State Projector (AGSP).
- Determined the upper bound of entanglement entropy for a quantum state upon application of AGSP.
- Qualitatively studied a variety of AGSPs including Detectability Lemma Operator, Polynomials of Hamiltonian, and Approximation of the Time Evolution Operator.



Indian Institute of Technology, Kharagpur,

Department of Physics,

Supervisor: Prof. Arghya Taraphder,

Jan-Apr 2021

Simulation of Quantum Many-Body Systems.

- Used PEPS ansatz to determine the ground state of the 2D Hubbard Model using Density Matrix Renormalization Group. The local diagonalizations were performed using the Lanczos algorithm.
- Simulated 1D Fermi-Hubbard model on an 8-qubit quantum computer and determined its ground state properties starting from the mean-field approximation using the Quantum Approximate Optimisation Algorithm.
- Reviewed literature on Topological Quantum Computation to understand the topological properties of anyons and the theory of braid groups. Studied superconducting systems that could support Majorana fermions.



Brown University,

The Rubenstein Group, Chemistry Department,

Supervisor: Prof. Brenda Rubenstein,

Apr-Aug 2020

Quantum Machine Learning on X-ray Scattering data.

- Demonstrated novel applications of Quantum Neural Networks on the molecular scattering data of NMM.
- Implemented Quantum State Preparation on Qiskit to encode classical information in qubits.
- Programmed Cartan's decomposition to simplify n-qubit Unitary operations into universal U3 & CNOT gates.
- Developed a Variational Quantum Machine Learning Algorithms on TensorFlow-Quantum.



The Australian National University,

Plasma Research Lab, Research School of Physics and Engineering,

Supervisors: Prof. James Sullivan, Dr. Daniel Cocks, Dr. Joshua Machacek,

May-Jul 2019

The Inverse Swarm Problem with Neural Networks.

- Employed the Mixture Density Networks to predict scattering cross sections from transport coefficients.
- Implemented Recurrent Neural Network to capture the mapping of the Inverse Swarm Problem.
- Used Variational Autoencoder to find the critical features characterizing the cross-sections.
- Simulated the Swarm problem with Boltzmann Equations using Numerical Methods and Parallel Algorithms.
- Presented my work at a seminar at the Research School of Physics and Engineering.



Sungkyunkwan University, South Korea,

Manybody Physics Lab, Department of Physics,

Supervisor: Prof. Jung Hoon Han,

May-Jul 2018

Machine Learning on two-dimensional Magnetic Spin Structures.

- Applied Convolution Neural Network to predict features of the spin phases of HDMZ Hamiltonian
- Accelerated Monte Carlo Simulations over the HDMZ model with Parallel Computing on CUDA.
- Implemented Unsupervised Machine Learning schemes like PCA and K-means Clustering.
- Worked on a variety of spin models, including Heisenberg, HDMZ, Ising, Pott's, XY, and Blume-Capel.
- Gave a talk on "Machine Learning in Physics" at the Department of Physics, SKKU.

Skills And Expertise

Programming Languages - Python, C/C++, MATLAB, Mathematica, Julia, & Fortran.

Scientific Programming Libraries - SciPy, NumPy, Matplotlib, CuPy & Pandas.

Quantum Computing and QML - Qiskit, Cirq, Tensorflow-Quantum, & PennyLane

Machine Learning and Deep Learning - TensorFlow, Keras, Pytorch, & Scikit-Learn.

Density Functional Theory - Avogadro, Gaussian, and Quantum Espresso.

Other Skills - Tensor Network (MPNUM & TeNPy), Parallel Programming (MPI & CUDA), Linux, & Git.

Miscellaneous

- **Teaching Assistant** in General Chemistry course (CHM 116) at Purdue University.
- **Qiskit Challenge India**, 2020: Completed the Quantum ML Challenge on Hackerearth.
- **Inter-IIT Tech Meet**, Roorkee, 2019: Presented my research at the Student Academic Conference
- **Hackerrank**: Won a Silver and four Bronze medals in various competitive coding contests.
- **National Service Scheme (NSS)**: I volunteered to work in NSS as a group leader for two years. I taught underprivileged students, organised free health check-up, and monitored road construction in remote villages. My unit won a gold medal in the Annual NSS Meet 2016.
- **Student Mentor Programme**: As a mentor, I guide newcomers and sophomores with their academics.