Ashish Kumar Patra

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Research Interests

Hybrid quantum-classical algorithms for molecular simulation, including machine-learning-assisted subspace expansion within density matrix embedding frameworks; resource-efficient primitives for early fault-tolerant quantum computing, spanning phase estimation and functional-transform algorithms; and quantum measurement and noise characterization, drawn from a background in continuous-variable quantum optics and hardware benchmarking on superconducting devices.

Education

M.Tech (Quantum Computing) **Aug. 2022 – May 2024**
Defence Institute of Advanced Technology, Pune *CGPA: 9.15/10*

M.Sc Physics **Jul. 2019 – Jun. 2021**
Loyola College, Chennai *CGPA: 8.44/10*

B.Sc Physics with Computer Applications **Jun. 2016 – Jun. 2019**
D.G. Vaishnav College, Chennai *CGPA: 8.7/10*

Work Experience

Quantum Analyst **Jul. 2024 – Present**
QClairvoyance Quantum Labs Pvt. Ltd.

- Built and **benchmarked a DMET–SQD quantum simulation pipeline** for ligand-like molecular Hamiltonians spanning **20–30 qubits**, using a fragment-based embedding strategy validated against DMET-FCI reference energies (arXiv:2511.22158).
- Carried out a large-scale experimental study of DMET-SQD on **IQM's Sirius 24-qubit superconducting processor** (up to **16 operational qubits**), combining SQD with the **Local Unitary Cluster Jastrow (LUCJ) ansatz** to estimate chemically accurate ground-state energies across a set of benchmark molecules (arXiv:2604.01983).
- Developed **QSCI-RBM**, a machine-learned compact subspace generation protocol using **Restricted Boltzmann Machines** within the DMET framework, trained on quantum-sampled configurations to target high-probability determinants. Applied to a **Carmofur–SARS-CoV-2 Mpro** protein-ligand complex on the **Fujitsu FX700** state-vector simulator, reaching chemical accuracy using only ∼4% of the configuration subspace versus ∼20% for standard SQD (arXiv:2606.30551, with an extended manuscript in preparation).
- Designed a **polylogarithmic-time quantum algorithm for the Laplace transform** via eigenvalue transformation techniques, developing a general framework for efficient functional evaluation on quantum computers and analyzing its resource scaling (arXiv:2512.17980).
- Contributed to **resource estimation** for VQE on small molecules, quantifying the impact of fermion mappings and Hamiltonian reductions on circuit depth; published in *Journal of Computational Chemistry* (DOI: 10.1002/jcc.70379).
- Contributed to a **DMET-VQE** framework using the **COMPASS ansatz**, a dynamically constructed, operator-commutativity-based state-preparation scheme for strongly correlated molecular systems, extending the applicability of embedded quantum simulations to larger, more complex chemical systems (arXiv:2604.19470).
- Reproduced and validated published complexity/runtime claims for quantum matrix-multiplication subroutines in Qiskit.

Publications & Preprints

- **Ashish Kumar Patra**, Anurag K. S. V., Ruchika Bhat, Sai Shankar P., Rahul Maitra, Jaiganesh G. *Machine-Learned Compact Subspace Generation for Quantum Selected Configuration Interaction within Density Matrix Embedding Framework*, arXiv:2607.20585 (Jul. 2026)
  Introduced QSCI-RBM, an RBM-based compact subspace generation protocol within DMET; applied to a Carmofur-Mpro (SARS-CoV-2 main protease) protein-ligand complex, reaching chemical accuracy with ∼4% of the configuration subspace versus ∼20% for standard DMET-SQD.

- **Ashish Kumar Patra**, et al. *Quantum Simulation of Ligand-like Molecules through Sample-Based Quantum Diagonalization in Density Matrix Embedding Framework*, arXiv:2511.22158 (Nov. 2025, **Accepted in JCP**)
  Built a fragment-based DMET-SQD pipeline achieving strong agreement with DMET-FCI benchmarks for 20-30 qubit molecular systems.

- Anurag K. S. V[†]., **Ashish Kumar Patra**[†] († equal contribution), et al. *Towards Chemically Accurate and Scalable Quantum Simulations on IQM Quantum Hardware: A Quantum-HPC Hybrid Approach*, arXiv:2604.01983 (Apr. 2026)
  Demonstrated DMET-SQD with the LUCJ ansatz on IQM's 24-qubit Sirius processor (up to 16 operational qubits); established practical limits of hybrid quantum-classical workflows via shot-dependent convergence analysis across benchmark molecules.

- Dibyendu Mondal, **Ashish Kumar Patra**, et al. *Advancing Practical Quantum Embedding Simulations via Operator Commutativity Based State Preparation for Complex Chemical Systems*, Chem.Sci. 2026 (Apr. 2026)
  Contributed to a DMET-VQE embedding framework using the dynamically constructed COMPASS ansatz for strongly correlated molecular systems.

- **Ashish Kumar Patra**, Saikumar Krithivasan. *Fractional Revival Dynamics in Kerr-Type Systems: Angular Momentum Moments and Classical Analogs*, arXiv:2601.09763 (Jan. 2026)
  Derived analytical revival structures using angular momentum moment methods; identified higher-order signatures of nonclassical evolution and their classical phase-space analogs.

- Mousumi Kundu, **Ashish Kumar Patra**, Anurag K. S. V., Ruchika Bhat, Sai Shankar P., Alok Shukla, Jaiganesh G. *An Analytically Trained Variational Surrogate for Quantum Phase Estimation on NISQ Hardware*, arXiv:2607.20943 (Jul. 2026)
  Trained a shallow Variational Quantum Circuit as an analytically grounded surrogate reproducing QPE measurement distributions for molecular ground-state energy estimation, circumventing the deep-circuit requirements of direct QPE on NISQ hardware.

- V., Anurag K. S., **Ashish Kumar Patra**, et al. *Resource Estimation for VQE on Small Molecules: Impact of Fermion Mappings and Hamiltonian Reductions*, *J. Comp. Chem.* 10.1002/jcc.70379 (Feb. 2025) **[Peer-reviewed]**

- Akash Kumar Singh, **Ashish Kumar Patra**, et al. *A Polylogarithmic-Time Quantum Algorithm for the Laplace Transform*, arXiv:2512.17980 (Dec. 2025)
  Designed a poly-log scaling algorithm via eigenvalue transformation; provides a general framework for efficient functional evaluation on quantum computers.

- **Ashish Kumar Patra**, et al. *Survey of Quantum Algorithms: Foundations, Frameworks and Applications*, Authorea preprint (Jun. 2025), DOI: 10.22541/au.176341037.72812424/v1

Research & Lab Experience

Balanced Optical Homodyne Detection — Aug. 2023 – May 2024

(guided by Dr. G. Raghavan and Dr. K. Raju Pandiri, DIAT)

- Designed and built a **95%-visibility Mach–Zehnder interferometer** for precision measurement of weak optical fields; signal level $\sim 10^{-5}$ relative to local oscillator—directly probing the quantum noise floor.
- Reconstructed Wigner functions and density matrices from homodyne statistics, performing full quantum state tomography for vacuum and weak coherent states.
- Developed a beamsplitter noise model and quantified how decoherence corrupts the interference structure carrying quantum information.
- Presented at ***ICQTA 2024*** and ***OPTOIn 2024***.

Two-Qubit Photonic Tomography (SPDC) — Jan. 2023 – Apr. 2023

(guided by Dr. K. Srinivasan and Dr. G. Raghavan, DIAT)

- Constructed a β-BBO SPDC source achieving $\sim$10% heralding efficiency for polarization-entangled photon pair generation.
- Performed **two-qubit quantum state tomography** using maximum-likelihood estimation (MLE); developed computational tools for density matrix reconstruction and entanglement quantification.

Revivals in Nonlinear Kerr Systems **Jan. 2021 – May 2021**

(guided by Mr. Saikumar K. and Mr. Joseph Prabagar, Loyola College)

- Derived analytical conditions for quantum revival and fractional revival under the Kerr Hamiltonian; computed higher-order observable moments as signatures of nonclassical dynamics with no classical counterpart.
- Constructed quantum carpets to visualize wavepacket dynamics and their classical phase-space correspondences.

Technical Skills

- **Quantum Hardware & Frameworks:** IBM Quantum, IQM Cloud, Qiskit, CudaQ, PennyLane, QuTiP
- **Algorithms & Methods:** VQE, QAOA, QPE, Trotterization, DMET, SQD, Quantum Tomography (MLE), Wigner Function Reconstruction, Error Mitigation
- **Programming:** Python (advanced), C/C++, MATLAB, JavaScript
- **Tools:** LaTeX, Git
- **Additional: Qutrit** – custom simulation framework for ternary quantum systems; implemented Deutsch–Jozsa, Simon's algorithm in qutrit gate model [GitHub]

Poster Presentations

- Balanced Homodyne Detection of CV Quantum States – ICQTA 2024
- High bandwidth homodyne detector development – OPTOIn 2024

Talks Delivered

- **"VQE – Theory and Implementation"** — Invited talk at the *Quantum Programming Bootcamp 2026*, held at QClairvoyance Quantum Labs in association with SVNIT.

Achievements

- Demonstrated B-92 QKD protocol using free-space single-photon transmission over a distance of 3 metres.

Languages & Tests

- **English** – TOEFL iBT: 112/120 (Reading: 24, Listening: 29, Speaking: 29, Writing: 30)
- **Odia** (Mother tongue), **Tamil** (Fluent), **Hindi** (Fluent)