Department of Chemical Sciences
Tata Institute of Fundamental Research,
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Curriculum Vitae

Amartya Bose

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Work Experience

2022 –	Assistant Professor, Tata Institute of Fundamental Research, Mumbai, India
2019 – 2022	Postdoctoral Research, Princeton University, Princeton, USA
2018 – 2019	Research Associate, University of Illinois at Urbana-Champaign, USA

Education

2012 – 2018	Ph. D. Chemistry, University of Illinois at Urbana-Champaign, USA	G. P. A. : 3.91/4
2007 – 2012	Integrated Master's in Chemistry, Indian Institute of Technology, Kanpur	G. P. A. : 9.30/10

Publications

[1] A. Bose, "QuantumDynamics.jl: A modular approach to simulations of dynamics of open quantum systems", The Journal of Chemical Physics **158**, 204113 (2023).

[2] A. Bose and P. L. Walters, "Impact of Solvent on State-to-State Population Transport in Multistate Systems Using Coherences", Journal of Chemical Theory and Computation **19**, 4828–4836 (2023).

[3] A. Bose and P. L. Walters, "Impact of Spatial Inhomogeneity on Excitation Energy Transport in the Fenna–Matthews–Olson Complex", The Journal of Physical Chemistry B **127**, 7663–7673 (2023).

[4] A. Bose, "Pairwise connected tensor network representation of path integrals", Physical Review B **105**, 024309 (2022).

[5] A. Bose, "Zero-cost corrections to influence functional coefficients from bath response functions", The Journal of Chemical Physics **157**, 054107 (2022).

[6] A. Bose and P. L. Walters, "A multisite decomposition of the tensor network path integrals", The Journal of Chemical Physics **156**, 024101 (2022).

[7] A. Bose and P. L. Walters, "Effect of temperature gradient on quantum transport", Physical Chemistry Chemical Physics **24**, 22431 (2022).

[8] A. Bose and P. L. Walters, "Tensor Network Path Integral Study of Dynamics in B850 LH2 Ring with Atomistically Derived Vibrations", Journal of Chemical Theory and Computation **18**, 4095–4108 (2022).

[9] A. Bose and N. Makri, "Quantum-classical path integral evaluation of reaction rates with a near-equilibrium flux formulation", International Journal of Quantum Chemistry **121**, 10 . 1002/qua . 26618 (2021).

[10] A. Bose and S. Torquato, "Quantum phase transitions in long-range interacting hyperuniform spin chains in a transverse field", Physical Review B **103**, 014118 (2021).

[11] A. Bose and P. L. Walters, "A tensor network representation of path integrals: Implementation and analysis", arXiv pre-print server arXiv:2106.12523 (2021), arXiv:2106 . 12523.

[12] A. Bose and N. Makri, "All-Mode Quantum–Classical Path Integral Simulation of Bacteriochlorophyll Dimer Exciton-Vibration Dynamics", The Journal of Physical Chemistry B **124**, 5028–5038 (2020).

[13] A. Bose and N. Makri, "Coherent State-Based Path Integral Methodology for Computing the Wigner Phase Space Distribution", The Journal of Physical Chemistry A **123**, 4284–4294 (2019).

[14] A. Bose and N. Makri, "Quasiclassical Correlation Functions from the Wigner Density Using the Stability Matrix", Journal of Chemical Information and Modeling **59**, 2165–2174 (2019).

[15] A. Bose and N. Makri, "Wigner Distribution by Adiabatic Switching in Normal Mode or Cartesian Coordinates and Molecular Applications", Journal of Chemical Theory and Computation **14**, 5446–5458 (2018).

[16] A. Bose and N. Makri, "Non-equilibrium reactive flux: A unified framework for slow and fast reaction kinetics", The Journal of Chemical Physics **147**, 152723 (2017).

[17] A. Bose and D. Goswami, "Investigating the science of few-cycle pulses on simple model systems", in *Advances in Laser Physics and Technology*, edited by M. Mohan, A. K. Maini, A. B. Bhattacharjee, and A. K. Razdan (Cambridge University Press, New Delhi, India, 2015) Chap. 3, pp. 37–52.

[18] A. Bose and N. Makri, "Wigner phase space distribution via classical adiabatic switching", The Journal of Chemical Physics **143**, 114114 (2015).

[19] A. Bose and D. Goswami, "Insignificance of Relative Time Delay between Photons for a Ultrafast Two-Photon Process", in 2012 International Conference on Fiber Optics and Photonics (PHOTONICS) (2012), pp. 1–3.

Research Experience

Assistant Professor at TIFR

- Designed and developed an **open-source Julia package** for simulations of dynamics in quantum non-adiabatic systems.[1]
- Developed a rigorous technique for identification of dynamical pathways in quantum transport processes in complex systems.[2]

Postdoctoral Research at Princeton University

- Explored quantum effects of transverse field on spin chains with long-range interactions that have disordered stealthy hyperuniform ground states using density matrix renormalization group (DMRG) with Prof. Salvatore Torquato.[10] Showed the possibility of generating order from disorder through quantum fluctuations in these spin systems.

Independent Work

- Developed a tensor network-based path integral method for solving system-solvent problems using Matrix Product States (MPS). This Tensor Network Path Integral (TNPI) is shown to be able to span much longer memory lengths and handle larger systems than previously possibly with very modest computational resources. We illustrated the method using an electron transfer and an exciton transfer example.[11]
- Established a novel pairwise connected tensor network representation for path integrals. This work generalizes the ideas from the MPS representation to a more flexible custom tensor network that manifestly captures the structure of the Feynman-Vernon influence functional, further illustrating the deep fundamental ties between tensor networks and path integrals.[4]
- Derived a series representation for the coefficients that capture the influence of the solvent on to the system in terms of the Kubo transform of the so-called "bath response function."[5]
- Developed a new multisite tensor network formalism for simulating extended quantum systems coupled to local dissipative environments like exciton transfer and charge transfer chains coupled with local vibrations. This MS-TNPI is a two-dimensional structure that, when evaluated yields the time propagated reduced density matrix of the entire extended system in the form of a matrix product state.[6]
- Explored the impact of thermal gradients on quantum transport in the Frenkel-Holstein model. Demonstrated for the first time, the possibilities of control using spatially inhomogeneous temperature profiles.[7]
- Studied the excitonic dynamics and absorption spectrum of a B850 ring using MS-TNPI accounting for the effects of atomistically derived protein and vibrational environments.[8]

Ph. D. Research

- Derived an approach to approximating the thermal correlation functions for mixed quantum-classical methods. It is shown that this method can exactly calculate rates of reactions for systems in atomistic environments.[9]

- Simulated exciton transfer in a chlorophyll dimer with all local vibrations present. The effects of static disorder on the resultant dynamics were analyzed.[12]
- Formulated a new exact numerical method for calculating multidimensional Wigner distributions for thermalized operators.[13]
- Derived a method for calculating correlation functions using stability matrices under the quasiclassical approximation. A very simple yet accurate approximation which is applicable for multidimensional systems is proposed.[14]
- Applied the adiabatic switching based Wigner method to atomistic Hamiltonians in normal mode coordinates and Cartesian coordinates. Calculated quasiclassical correlation functions and explored the importance of Zero-Point Energy and quantization of the thermal density.[15]
- Constructed a nonequilibrium reactive flux based method for calculating rates of reactions. This method is shown to unify slow and fast reaction dynamics.[16]
- Described an efficient classical trajectory based method for calculating the quantum Wigner phase-space distribution.[18]

Master's Research Projects

- Investigated a simple model of two-photon processes using non-relativistic quantum electrodynamics.[19]
- Modelled and studied the impact of the shape of the envelope of a few-cycles laser pulse on the nature of the breakdown of rotating wave approximation in the dynamics of two-level systems.[17]
- Learned ultrafast spectroscopy with Prof. Debabrata Goswami. Worked on the instrumentation of a 2D nonlinear optical spectroscope using an acousto-optical modulator pulse shaper with colinear pulses.
- Worked with Prof. Martin Gruebele on expressing PGK-FRET proteins for subsequent study of protein dynamics in presence of gold nanorods during the Summer, 2011.

Conference Talks and Posters

August 2023	Talk on "Dynamics of Extended Open Quantum Systems — Tensor Network Path Integral Approaches" at Harish-Chandra Research Institute as a part of their Physics Colloquium series
July 2023	Talk on "Excitonic Dynamics: Path Integrals and Tensor Networks" at Kaleidoscope, 2023 at Udaipur
September 2022	Talk on "Non-Equilibrium Quantum Dynamics: Tensor Network Path Integral Formalism" at QMat 2022 hosted by Indian Institute of Technology Kanpur
Spring 2021	Talk on "Nuclear Quantum Effects in *ab initio* Water Dynamics" at American Physical Society's March Meeting
Summer 2019	Poster on "Classical and Path Integral Methods for Computing the Wigner Distribution" at American Conference of Theoretical Chemistry
Summer 2019	Poster on "Quantum-Classical Path Integral: Harmonic Backreaction & Blip Decomposition" at American Conference of Theoretical Chemistry
Summer 2017	Poster on "Quantum Mechanical Rate Calculations in Condensed Phase Reactions" at American Conference of Theoretical Chemistry
Summer 2017	Talk on "Quantum Mechanical Rate Calculations in Condensed Phase Reactions" at Midwest Theoretical Chemistry Conference
Spring 2016	Talk on "Wigner Phase Space Distribution via Classical Adiabatic Switching" at American Chemical Society's Annual Meeting

Teaching Experience

Fall 2023	Quantum Mechanics I
Spring 2023	Chemical Dynamics covering Time-dependent perturbation theory, Born-Oppenheimer approximation and non-Born-Oppenheimer processes, Gaussian wavepacket dynamics, quantum thermodynamics, ring polymer-based methods, etc.

Honors and Awards

2018	Certificate of Graduate Specialization in Computational Science and Engineering, UIUC
2017	Center for Advanced Theory and Molecular Simulation Travel Award, Department of Chemistry, UIUC
2016	Eastman Travel Award, Department of Chemistry, UIUC
2015 – 2016	Harry G. Drickamer Fellowship, Department of Chemistry, UIUC
2014 – 2015	Robert Carr Fellowship, Department of Chemistry, UIUC
2013 – 2014	Walter Brown Fellowship, Department of Chemistry, UIUC
2007 – 2012	KVPY Fellowship, Department of Science and Technology, Government of India: Fellowship instituted to promote excellence in pure science
2012	IIT Kanpur, Best Master's Thesis Dissertation
2008 – 2009	IIT Kanpur, Academic Excellence Award
2006	All India Rank 82 in the 5^{th} National Cyber Olympiad
2004	Qualified for the Indian National Mathematical Olympiad with qualifying rank 18; among 3 students from 10^{th} standard to qualify
2004	All India Rank 31 in Senior Mathematical Olympiad
2003	All India Rank 28 in Junior Mathematical Olympiad