USHNISH RAY

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Canada

## EDUCATION

- *Ph.D.* in Physics, University of Illinois at Urbana-Champaign, September 2008 – May 2015
- *B.A. summa cum laude* with *High Honors* in Physics & *High Honors* in Computer Science Colgate University, September 2004 – May 2008

## EXPERIENCE

- *Consultant*, Quantum Create, October 2020 - present
- *Postdoctoral Research Scholar*, California Institute of Technology, July 2016 - July 2020
- *Postdoctoral Research Scholar*, Princeton University, September 2015 - July 2016
- *Research Assistant*, University of Illinois at Urbana-Champaign, June 2010 - May 2015
- *Teaching Assistant*, Physics Department at the University of Illinois at Urbana-Champaign, January 2010 – May 2010
- *Research Assistant*, University of Illinois at Urbana-Champaign, September 2008 – December 2009
- *Teaching Assistant*, Colgate University Physics Department, September 2005 – May 2008
- *Teaching Assistant*, Colgate University Computer Science Department, January 2005 – May 2008
- *Summer Researcher*, Colgate University Physics Department, June 2007 – August 2007
- *Summer Researcher*, Colgate University Physics Department, June 2006 – August 2006
- *Network Security and Software Development Consultant*, Stadmed Pvt. Ltd (India), 2002-2003
- *Software developer* for St. James' School, Calcutta 2001-2002

## SELECTED AWARDS & MEMBERSHIPS

- *University of Illinois at Urbana-Champaign Fellowship*, September 2008
- *Physics and Astronomy Alumni Award*: Colgate, April 2008
- *Award* for Academic Excellence in Computer Science: Colgate, April 2008
- *Charles A. Dana Scholar*: Colgate, 2006-2008
- *Phi Beta Kappa*: Colgate, September 2007
- *Schlichting Student Researcher*: Colgate, May 2007
- *Extraordinary Talent in Computing*: State-wide Telegraph School Awards, Calcutta 2003, from among over 100,000 high-school students in West Bengal.

## PROFESSIONAL SERVICE

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| *Referee Service:* | Physical Review Letters, Physical Review A, B & E, and Journal of Chemical Physics. |
| *Consulting Service:* | Stadmed Pvt. Ltd., Chaos Alchemists, & Misfit Venture Partners. |

## ADVISING & MENTORSHIP

*Former Graduate Students:*

- Bruno Ricardi de Abreu
- Phillip Helms
- Zhihao Cui
- Chong Sun

## TECHNICAL SUMMARY

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|---|---|
| *Programming Languages:* | C/C++, Java, Fortran, Python, Matlab, Visual Studio, Objective C, Assembly Language |
| *Parallel Frameworks:* | OpenMP, POSIX, MPI, CUDA |
| *Research Libraries:* | *GSL, ARPACK++, LAPACK, BOOST, QMCPACK, ITENSOR, MOLPRO, PYSCF, BLOCK, CERES* |
| *Other:* | Mathematica, XCODE, Eclipse, Linux, Windows, MacOS, Git, SVN, SQL, Oracle, UML |

## SOFTWARE

The following libraries are state-of-the-art computational frameworks that I designed and implemented from the ground up to study various systems over the course of my career.

- *pyRET:* Implements Density Matrix Embedding Theory (DMET) for strongly correlated systems. It is being used to study ground state properties of d-wave superconductors and magnetism at finite temperatures. It can be extended to study a range of other systems including topological insulators.

- *VANSS:* Variational algorithm for nonequilibrium stationary states uses the variance minimizing principle to optimize guiding distribution functions that are used by CANSS to mitigate variance growth problems.

- *CANSS*: Cloning algorithm based code used to calculate large deviation functions and associated cumulants for a variety of systems on the lattice and in the continuum. It has extensions for stochastic MD type of simulations to study phenomena in realistic materials, such as heat flow in carbon nanotubes.

- *CSSER*: Stochastic Series Algorithm based code to study sign-free problems on the lattice. Massive systems — more than 500,000 particles — can be addressed in many different settings. It has been used to study disordered systems and ultra-cold atomic gases.

## RESEARCH HIGHLIGHTS

- *Devised an importance sampling strategy for calculating large deviation functions and cumulants of nonequilibrium systems via Monte-Carlo strategies. Also, outlined a generalized variational principle that can be used to systematically construct guiding distribution functions needed for importance sampling.* Published in *Physical Review Letters.*

- *Performed the largest state-of-the-art calculations for disordered quantum systems to date that identified the Superfluid-Bose-glass phase transition in collaboration with experiments.* Published in *Nature Physics* as front-cover article.

- *Identified the origin of metastability in Bose-Einstein condensates in optical lattice experiments. Large-scale simulations with 200,000 particles were performed to calculate finite temperature properties of strongly correlated superfluids.* Published in *Physical Review A* and selected as *Editor's Pick.*

## PUBLICATIONS

(* indicates co-first authorship, names arranged alphabetically.)

1. Ushnish Ray and David Limmer, "Importance Sampling Large Deviations in Non-equilibrium Steady States: Part 2", *in preparation* (2020).

2. Zhi-Hao Cui, Chong Sun, Ushnish Ray, Bo-Xiao Zheng, Qiming Sun, Garnet Kin-Lic Chan, "Ground-state phase diagram of the three-band Hubbard model in various parametrizations from density matrix embedding theory", *Phys. Rev. Research* 2, 043259 (2020).

3. Mario Motta, Claudio Genovese, Fengjie Ma, Zhi-Hao Cui, Randy Sawaya, Garnet Kin-Lic Chan, Natalia Chepiga, Phillip Helms, Carlos Jiménez-Hoyos, Andrew J Millis, Ushnish Ray, Enrico Ronca, Hao Shi, Sandro Sorella, Edwin M Stoudenmire, Steven R White, Shiwei Zhang, "Ground-state properties of the hydrogen chain: Dimerization, insulator-to-metal transition, and magnetic phases", *Phys. Rev. X* 10, 031058 (2020).

4. Kiel T. Williams, Yuan Yao, Jia Li, Li Chen, Hao Shi, Mario Motta, Chunyao Niu, Ushnish Ray, Sheng Guo, Robert J. Anderson, Junhao Li, Lan Nguyen Tran, Chia-Nan Yeh, Bastien Mussard, Sandeep Sharma, Fabien Bruneval, Mark van Schilfgaarde, George H. Booth, Garnet Chan, Shiwei Zhang, Emanuel Gull, Dominika Zgid, Andrew Millis, C. J. Umrigar, Lucas K. Wagner, "Direct comparison of many-body methods for realistic electronic Hamiltonians", *Phys. Rev. X* 10, 011041 (2020).

5. Ushnish Ray and Garnet Kin-Lic Chan, "Constructing Auxiliary Dynamics for Nonequilibrium Stationary States by Variance Minimization", *J. Chem. Phys.* 152, 104107 (2020). (**Selected as Editors' picks and website front-page article, March 12, 2020.)**

6. Chong Sun, Ushnish Ray, Zhi-Hao Cui, Miles Stoudenmire, Michel Ferrero and Garnet Kin-Lic Chan, “Finite temperature density matrix embedding theory”, *Phys. Rev. B* 101, 075131 (2020).

7. Ushnish Ray and David Limmer, "Heat current fluctuations and anomalous transport in low-dimensional carbon lattices”, *Phys. Rev. B* 100, 241409(R) (2019). (**Selected for Rapid Communication.**)

8. Phillip Helms, Ushnish Ray, and Garnet Kin-Lic Chan, “Dynamic phase behavior of the single- and multi-lane asymmetric simple exclusion process via matrix product states”, *Phys. Rev. E* 100, 022101 (2019).

9. Bruno R. de Abreu, Ushnish Ray, Silvio A. Vitiello, David Ceperley, “Properties of the Superfluid in the Disordered Bose-Hubbard Model”, *Phys. Rev. A* 98*,* 023628 (2018).

10. Ushnish Ray, Garnet Kin-Lic Chan, David T. Limmer, “Exact Fluctuations of Nonequilibrium Steady States from Approximate Auxiliary Dynamics”, *Phys. Rev. Lett.* 120, 210602 (2018).

11. Ushnish Ray, Garnet Kin-Lic Chan and David Limmer, “Importance Sampling Large Deviations in Non-equilibrium Steady States: Part 1”, *J. Chem. Phys.*, 148 (12), 124120 (2018). (**Selected as Editors’ picks and website front-page article, March 29, 2018.)**

12. Mario Motta, David M. Ceperley, Garnet Kin-Lic Chan, John A. Gomez, Emanuel Gull, Sheng Guo, Carlos Jimenez-Hoyos, Tran Nguyen Lan, Jia Li, Fengjie Ma, Andrew J. Millis, Nikolay V. Prokof'ev, Ushnish Ray, Gustavo E. Scuseria, Sandro Sorella, Edwin M. Stoudenmire, Qiming Sun, Igor S. Tupitsyn, Steven R. White, Dominika Zgid, Shiwei Zhang, “Towards the Solution of the Many-Electron Problem in Real Materials: Equation of State of the Hydrogen Chain with State-of-the-Art Many-Body Methods”, *Phys. Rev. X* 7, 031059 (2017).

13. Carolyn Meldgin*, Ushnish Ray*, Phillip Russ, David Chen, David Ceperley and Brian DeMarco, “Probing the Superfluid to Bose-glass Transition using Quantum Quenches of Disorder”, *Nature Phys.*, 12, 10.1038 (2016). (**Selected as front cover of Nature Physics July 2016.)**

14. Ushnish Ray, “Properties of Dirty Bosons in Disordered Optical Lattices”, *Doctoral Dissertation*, University of Illinois at Urbana-Champaign (2015).

15. David McKay*, Ushnish Ray*, Stefan Natu, Phillip Russ, David Ceperley and Brian DeMarco, “Metastable Bose-Einstein Condensation in a Strongly Correlated Optical Lattice”, *Phys. Rev. A* 91, 023625 (2015). (**Selected as Editors’ Suggestion.**)

16. Ushnish Ray and David Ceperley, “Revealing the Condensate and Non-condensate Distributions in the Inhomogeneous Bose-Hubbard Model”, *Phys. Rev. A* 87, 051603R (2013). (**Selected for Rapid Communication.**)

17. Ken Segall, Dan Schult, Ushnish Ray, Toshiro Ohsumi, “Numerical simulation of thermal noise in Josephson circuits”, *arXiv:*1110.0172 (2011).

18. Seo Ho Youn, Mingwu Lu, Ushnish Ray, and Benjamin L. Lev, “Dysprosium magneto-optical traps”, *Phys. Rev. A* 82, 043425 (2010).

19. E. J. Galvez, M. Malik, B. Melius, B. Gadway, and U. Ray, "Measurements of Phase Correlations between Polarization-Entangled Photons”, *International Conference on Quantum Information*, OSA Technical Digest (CD), Optical Society of America, paper JWC46, (2007).

## GRANTS AND RESEARCH ALLOCATIONS

- Quantum Simulations of Molecular and Solid State Systems, MCA93S030, XSEDE (2016).
  - Valued of awarded resources: $202,521.21

## INVITED TALKS

- Constructing approximate Auxiliary Dynamics for Nonequilibrium Stationary States, MoISSI workshop, Caltech; June 29, 2018.
- Large Deviation Approach to Nonequilibrium Stationary States, Caltech; December 4, 2017.
- Exploring the Superfluid-Bose-glass transition and their properties with SSE, Workshop on Understanding Quantum Phenomena with Path Integrals: From Chemical Systems to Quantum Fluids and Solids, The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy; July 3-7, 2017.
- Dirty Bosons in Disordered Optical Lattices, APS March Meeting; March 15, 2016.
- Probing the Superfluid Bose-glass transition using dynamical and equilibrium measurements, Electronic Structure Interest Group, University of Illinois; September 2014.
- QMC Studies of OLE with Disorder, Annual Review of DARPA Optical Lattice Emulator Program; February 2, 2014.
- QMC Studies of the Experimentally Realized 3d Disordered Bose-Hubbard Model, Electronic Structure Interest Group, University of Illinois; April 24, 2013.

## CONFERENCE PRESENTATIONS

- Quantum Algorithms for Quantum Chemistry and Materials, Washington DC, January 21-24, 2019
- Constructing guiding distribution functions with Variational Monte-Carlo, UC Berkeley Statistical Mechanics Meeting, January 10, 2017.
- Importance sampling large deviations in non-equilibrium steady states, Gordon Research Conference: Chemistry and Physics of Liquids, August 7, 2017.
- Efficient Strategies to Access Large Deviation Functions of Stationary Non-equilibrium States, UC Berkeley Statistical Mechanics Meeting, January 13, 2017. (**Received 1st Prize for the Poster Presentation.***)*
- Probing the Bose-glass-Superfluid phase boundary using quantum quenches of disorder in an optical lattice, APS DAMOP, June 4, 2014.
- Simulations of Bose-Hubbard Model, DARPA OLE, December 7, 2011.
- Progress toward the magneto-optical trapping of Dysprosium, APS DAMOP, May 20, 2009.
- Numerical simulation of flux on dynamics in a Josephson junction array, APS March Meeting, March 11, 2008.