Shivesh Pathak

Curriculum Vitae

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Education

Ph.D., Physics, University of Illinois at Urbana-Champaign, Expected graduation: May 2021
Expected dissertation: Accurate low-energy states and interacting effective models using *ab initio* quantum Monte Carlo

B.S., Physics, University of Illinois at Urbana-Champaign, 2016

Research Interests

Strongly correlated condensed matter systems, *ab initio* simulations of strongly correlated quantum systems, model development for strongly correlated electronic systems, massive scale computation and data science

Peer-Reviewed Journal Publications

S. Pathak *et al.* "Excited states in variational Monte Carlo using a penalty method", *J. Chem. Phys.* **154** (2021). (https://doi.org/10.1063/5.0030949)

S. Pathak, L.K. Wagner, "A light weight regularization for wave function parameter gradients in quantum Monte Carlo", *AIP Advances* 10 (2020). (https://doi.org/10.1063/5.0004008)

S. Pathak, L.K. Wagner, "Non-orthogonal determinants in multi-Slater-Jastrow trial wave functions for fixed-node diffusion Monte Carlo", *J. Chem. Phys.* 149 (2018). (https://doi.org/10.1063/1.5052906)

J.T. Uhl, **S. Pathak** *et al.* "Universal Quake Statistics: From Compressed Nanocrystals to Earthquakes," *Scientific Reports* **5**, 16493 (2015). doi:10.1038/srep16493. (http://www.nature.com/articles/srep16493)

Conference Presentations

S. Pathak *et al.* "Excited states in variational Monte Carlo using a penalty method", APS March Meeting 2021.

W. Wheeler, **S. Pathak,** J. Rodrigues, C. Lorsung, Y. Chang, Y. Zhou, B. Busemeyer, K. Williams, A. Munoz, L.K. Wagner, "PyQMC: an all-Python real-space quantum Monte Carlo code", APS March Meeting 2021.

B. Busemeyer, J. Rodrigues, **S. Pathak,** L. K. Wagner, "An approach to discovering the low-energy space for effective quantum models of realistic systems", APS March Meeting 2020.

W. Wheeler, **S. Pathak,** L.K. Wagner, "Fitting effective models using QMC parameter derivatives", APS March Meeting 2019.

S. Pathak, L.K. Wagner, "Non-Orthogonal Determinant Multi-Slater-Jastrow Wave Functions in QMC", APS March Meeting 2018.

S. Pathak, L.K. Wagner, "Implementing orbital optimization of quantum Monte Carlo wavefunctions in QWalk", National High Magnetic Field Laboratory Theory Winter School 2017.

Honors and Awards

Teacher Ranked as Excellent, University of Illinois at Urbana-Champaign, 2016-2019
University of Illinois at Urbana-Champaign University Fellowship, 2019
Phi Beta Kappa Honor Society, 2016
Golden Key International Honor Society, 2016
Summa Cum Laude, University of Illinois at Urbana-Champaign, 2016
Lorella M. Jones Summer Research Award,
University of Illinois at Urbana-Champaign, 2014
University Achievement Scholarship,
University of Illinois at Urbana-Champaign, 2013–2016

Research Experience

Doctoral Research

Graduate Researcher, University of Illinois at Urbana-Champaign**,** 2016 – Present
Use of the supervised machine learning framework Density Matrix Downfolding and *ab initio* quantum mechanics simulations in model Hamiltonian development and computation of low-energy excited states for quantum systems on high dimensional Hilbert spaces
Complete: Low-energy spectrum of benzene,
non-interacting model for single layer graphene with lattice effects
In progress: Non-interacting model for bilayer graphene with lattice effects
Model with long-range density-density interactions for graphene
Development of highly parallel real space *ab initio* quantum Monte Carlo codes: QWalk in C++, PyQMC in Python (https://github.com/QWalk, https://github.com/WagnerGroup/pyqmc)

Graduate Intern, Lawrence Livermore National Lab, 2017
Development of distributed sparse matrix operations on massively parallel quantum simulation code using C++
The code was used for massive scale *ab initio* density functional theory calculations

Graduate Intern — Lawrence Livermore National Lab, 2016
Development and testing for a massively parallel code hydrodynamics code Miranda using FORTRAN 2003 with C/C++ interoperability and Lua interfacing.
Testing was on massive scale simulation of shock waves in stellar gas environments

Pre-Doctoral Research

Undergrad Researcher, University of Illinois at Urbana-Champaign, 2013 – 2016
Data analysis and function fitting for experimental slip avalanche data from nanopillars to earthquakes
Study determined that a theoretical model for universality of slip avalanches describes slip events seen in reality

Teaching Experience

Teaching Assistant — University of Illinois at Urbana-Champaign, 2016 – 2019
Taught PHYS 212, PHYS 213/214 and PHYS 436
"Teacher Ranked as Excellent" all five semesters, evaluated by Illinois Center for Innovation in Teaching & Learning

Engagement

Wesley Food Pantry Board Member and Volunteer, 2017 – Present
Graduate Employees Organization Steward, 2018 **–** Present

Languages

Fluent in English and Hindi, Spanish competency