Quantum Monte Carlo many-body methods: introduction and recent progress

Professor Mita’s talk will give a brief introduction into the electronic structure quantum Monte Carlo (QMC) based on sampling of particles coordinates. Application examples encompass strongly correlated systems, molecules, ultracold atomic condensates, etc. So far, however, such QMC calculations have been limited to static, collinear treatment of electronic spins. Recently, we have developed QMC with variable spins for calculations that involve spin-orbit or other spin-dependent Hamiltonians and this will be illustrated on several examples.

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Professor Mitas joined the NC State Department of Physics after spending several years as a theorist at the National Center for Supercomputing Applications, University of Illinois. He is a member of the Center for High Performance Simulation specializing in computational and theoretical approaches for nanoscience/materials, biomolecular and quantum systems. His work includes many-body computational methods such as quantum Monte Carlo simulations of electronic structures. He is known for pioneering high-accuracy calculations of atoms, molecules, clusters and solids, analysis of many body nodes of fermion states and applications of pairing wave functions to electronic structures. He has also been co-developer of multi-dimensional spatial interpolation and landscape processes methods for modeling, visualization and simulations of geospatial processes.

Monday, October 26, 2020
4:00 pm
Virtual Zoom Seminar
For more information on the Zoom link, please email Allison Dzubak – adzubak@bowdoin.edu