School in Computational Condensed Matter Physics:
From Atomistic Simulations to Universal Model Hamiltonians

Quantum Monte Carlo simulations of spin systems

Anders W. Sandvik, Boston University

Lecture 1: Stochastic series expansion method for simulations of quantum spins

Lecture 2: Ground-state projection of quantum spins in the valence bond basis

Lecture 3: Systematic finite-size scaling methods for analyzing critical points

Lecture 4: Out-of-equilibrium quantum Monte Carlo simulation and quantum annealing

Abstract: In these lectures I will give an overview of quantum Monte Carlo (QMC) methods and their applications, focusing on bipartite quantum spin systems where the "sign problem" is avoided and very large system sizes can be reached. The stochastic series expansion (SSE) method is a standard tool for simulations at non-zero temperature, and the ground state can also be obtained by going to temperatures much lower that the finite-size gap of the system studied. Many quantities suitable for characterizing ordered and disordered states can be calculated. An alternative way to study the ground state is to apply a "projector" which filters out the ground state, e.g., a high power H^n of the Hamiltonian, to an initial "trial state". For spin systems, such a scheme can be formulated in the basis of valence bonds (singlet pairs), which has the advantage of enforcing a given total-spin quantum number S and momentum from the outset, which improves the convergence properties. By including unpaired spins in $S > 0$ states one can also obtain unique information on the nature of the low-energy excitations; specifically one can study spinons and their bound states. After introducing the SSE and ground-state projector QMC methods I will discuss applications to systems with quantum-critical points. I will discuss finite-size scaling methods for extracting the critical coupling and critical exponents in a systematic, unbiased fashion. The last lecture will be devoted to a recently developed method to simulate systems out of equilibrium, with a time-evolving Hamiltonian. Schrödinger dynamics can be implemented in simple generalizations of ground-state projector QMC methods. While imaginary-time dynamics is of course different from real-time dynamics, it turns out that one can obtain some useful information on real-time dynamics from imaginary time. In particular, in a linear ramp of an interaction with velocity v, close to the adiabatic limit the differences of the two are only of order v^3. Therefore, imaginary-time QMC simulations can be used to investigate the ability of quantum annealing protocols to reach complex ground states, which is of interest in the context of the quantum adiabatic paradigm for quantum computing. I will discuss the method and applications to quantum spin glasses.