Loop Cluster Monte Carlo Simulation of Quantum Magnets Based on Global Union-find Algorithm

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Why quantum lattice models?

- QMC: quantum spin models, bosonic Hubbard models, etc
- Global union-find algorithm
- Effective for large systems
- various types of long-range order
- Quantum disordered phase transition, phase diagram of quantum magnets
- Quantum critical point

Impurity induced long-range order

- Quantum fluctuations and impurities
- Quantum critical point
- Quantum critical fluctuations
- Quantum impurities

The ALPS Project

- Open source libraries and simulation code for strong correlated quantum systems
- Quantum Monte Carlo
- Exact diagonalization
- Dynamical mean field theory
- Density matrix renormalization group

Motivation

- Established algorithms
- Enhanced formalism for applicable simulations from theory and experiment

ALPS framework and Peta-scale Supercomputers

- Open source libraries and simulation code for strongly correlated quantum systems
- Quantum Monte Carlo, worm algorithm, etc
- Field-theoretical models, Bose-Hubbard model, etc
- Bosonic Hubbard models, etc
- QLM: Quantum spin models, quantum liquids, bosonic Hubbard models, etc

What is quantum Monte Carlo?

- Variational Monte Carlo (Gros, White, Nishino, Schollwoeck)
- Dynamical mean field theory
- Density matrix renormalization group (Salapino, Hirsh, Sorella, Imada)
- Weak 1st order phase transition?
- Between long-range ordered phase with incompatible symmetries (or supersolid: co-existence of diagonal and off-diagonal order in quantum vibronics)

World-line QMC for lattice models

- Progress since 1990s
- Glauber update in imaginary time
- String method in QMC simulation
- Slow down problem in MCMC

Continuous imaginary-time loop algorithm

- Representation of a quantum system as an n-dimensional classical system
- Binary tree algorithm for cluster identification

Parallelization of loop algorithm

- Distributing world-line configurations to several processors
- Binary tree algorithm for cluster identification
- Extreme parallelism

Multiple-level parallelization

- Parallelization within one Monte Carlo step
- Exchange Monte Carlo (parallel tempering)
- Path integral renormalization
- Random averaging or quenched disorder
- Improvement in the performance of the multi-level parallelization

QMC Simulation by the K computer

- Minimum QMC calculations of S=5/2 antiferromagnetic Heisenberg chains
- Coordinate length: 200,000, energy gap: 0.04005
- Identification of connected components of large-scale graph

- Number of subchains: 10^9, number of clusters: 10^9
- Study of fundamental problems in quantum statistical physics not by linear combination but by the parallel graph operations
- Achieved same size as "large phase transition" problems in cold-dense systems
- Speed up by hybridization
- Achieved speedup of 10^5