Term Project Proposal (Phys 580)

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Quantum Spin Systems:

One key target of theoretical physics is to give the simplest model for explaining many kinds of complex phenomena. In the context of condensed matter physics, spin systems play this role. By studying Ising model, classical thermal phase transitions and critical phenomena have been fully understood. Recently, quantum spin systems have been forming the theoretical framework for studying exotic ground states and quantum phase transitions. Because of many possible ordered or disordered ground states and diverse excitations, quantum spin systems give us a better access to quantum collective behaviours. [1][2]

Nowadays, one of the most important research fields is to study nonuniform or frustrated spin systems, which give disordered ground states. Quantum spin systems are also closely related to quantum information theory[3]. For example, some concepts in quantum many-body physics, such as entanglement entropy, can be used to describe the ground states of quantum spin systems[4]. Heisenberg interaction is the most essential spin coupling, often as a start point for understanding magnetic materials.

Computational Tools:

Most quantum spin systems cannot be solved exactly. Some of them can be studied based on approximations or assumptions. But their validity still needs verifying. So pure numerical study of the Hamiltonian itself is necessary. Exact diagonalization (ED), quantum Monte Carlo (QMC), and density-matrix renormalization group (DMRG) are basically the most important computational tools for quantum systems. The basic idea of ED is to build the matrix for Hamiltonian and then diagonalize it. Any information of the system can be extracted from the eigenvalues and eigenstates. GNU Scientific Library and LAPACK supply good routines of diagonalization. However, because the size of Hilbert space grows exponentially as the system size, ED can just study small systems. Large-scale Monte Carlo simulation[5] is widely used but it cannot simulate the frustrated systems or fermion systems. Last but not least, DMRG is a powerful computational tool. Using it, large systems can be studied and there is no sign problem. But the major drawback is that it displays its full force mainly for one-dimensional systems[6]. The fundamental idea of DMRG is to reduce the size of the Hilbert space by replacing the lattice sites by the energy levels in the renormalization-group framework.

Plans and Expectations:

I am interested in computational condensed matter physics. I have much experience in both ED and QMC. It will be very important for me to master another key computational tool. So the main target of this term project is to understand DMRG theory, to master this technique, and to apply it to simple models. In September, I will read about DMRG[6], understanding it and knowing how to realize it numerically. In October, DMRG will be used to study the Heisenberg models (both $S=1/2$ and $S=1$) and I will write codes for it. $S=1/2$ and $S=1$ models have totally different properties and it can be verified numerically[7]. Ground state energy, energy gap between the ground state and the first-excited state, and correlation functions are to be measured. I often use C but I will try to code it up using C++ this time. In early November, results will be obtained by running the codes. Based on these results, I will give an oral presentation in mid November. I will spend another two weeks finishing the final report.

References:

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[5] A. W. Sandvik, Ground State Projection of Quantum Spin Systems in the Valence Bond-Basis, Phys. Rev. Lett. 95, 207203(2005).
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[7] S. R. White and D. A. Huse, Numerical renormalization-group study of low-lying eigenstates of the antiferromagnetic S=1 Heisenberg chain, Phys. Rev. B 48, 3844(1993) .