Generalizations of Density matrix Renormalization Group methods

Efficient simulation of one-dimensional quantum many-body systems
Author: G.Vidal

Renormalization algorithms for Quantum-Many Body Systems in two and higher dimensions
Authors: F. Verstraete, J. I. Cirac

Recommended with a Commentary by Steve White, University of California, Irvine.

The density matrix renormalization group (DMRG), has proven to be extremely effective in simulating 1D quantum systems, and 2D strips of modest width. Generalizations and improvements to DMRG have also been developed. Reasonably efficient methods for extracting spectral functions have been devised, and other generalizations utilizing transfer matrices allow finite temperature studies in translationally invariant quantum chains and 2D classical spin systems. It was found that the DMRG wavefunction can be written in a matrix product form very similar to (i.e. generalizing) the Affleck-Kennedy-Lieb-Tasaki (AKLT) state of spin-1 antiferromagnetic chains. DMRG has also proven useful in quantum chemistry.

A method for true 2D quantum simulations has been the holy grail for DMRG, but until recently, there were no credible ideas of how one might do it.

Meanwhile, the field of quantum information has been developing. Part of the work in this field is tied in with trying to build a quantum computer, or program one, but another part seeks to understand basic ideas of entanglement in interacting quantum systems and how one might exploit entanglement to do useful things. A collection of techniques and ways of understanding quantum systems have been devised. However, the usefulness of this work had not been clear, with quantum computers still just a possibility for the future.

In the last two years researchers on quantum information have realized that many of their techniques and tricks can apply to the simulations of quantum lattice systems. These techniques turn out to be closely related to DMRG. The first advance was Vidal's development of an algorithm allowing the efficient solution of the (real) time-dependent Schrodinger equation in a 1D quantum system. Here the trick was to use the Trotter decomposition and to adapt the basis as the system evolves. Vidal's algorithm is very important but is based on matrix product states; it fits naturally into a DMRG framework, and might easily have been discovered without input from the quantum information community. New algorithms developed since then have been much more surprising.

The most surprising approach I've heard has been in a talk by Verstraete, but the paper unfortunately hasn't been finished yet. This is a new way to simulate disordered 1D systems. A single realization of a disordered quantum chain can be

efficiently simulated with traditional DMRG. Verstraete and Cirac developed an approach to simulate all realizations of a disordered chain in one simulation! A set of auxilliary sites (ancilla) are introduced, one for each real site, and these ancilla are entangled with the real sites. Hamiltonian terms are introduced which encode the various disorder realizations into interactions with the ancilla. Starting with the nondisordered ground state, the interactions are slowly turned on in an adiabatic time evolution, producing a single quantum state which, when the ancilla are traced out, gives the average of all ground states over the realizations of disorder.

Another dramatic development by Verstraete and Cirac is the generalization of the matrix product state to a tensor product state to describe systems in 2D or 3D. The key idea is to make a tensor for each site which has an index associated with each near-neighbor link, and one index labeling the states of the site. When all the tensors are traced out over all the links, the remaining state indices give the wavefunction. This can give a remarkably compact representation for a 2D wavefunction. The algorithm to optimize this tensor product and calculate its energy and properties is clever and complicated. In its still early stage of development it has already allowed simulations of 20x20 Heisenberg systems--small by quantum Monte Carlo standards but much bigger than can be accomplished by a standard "strip" DMRG algorithm. While this system can be studied by QMC, frustrated and fermion systems give the minus sign problem, which does not plague DMRG. Perhaps the holy grail, reliable, accurate, and unbiased simulations of large 2D fermion clusters, is becoming within reach!