Homework 6: Due May 17

Entanglement and Tensor Networks, Spring 2016, Prof. White

1. **Quantum Number DMRG with ITensor**

We will explore differences between DMRG calculations which do or do not conserve quantum numbers. If you have not done so already, download and install ITensor. Go into the sample/ folder under the folder containing the ITensor source code.

Read through the files dmrg.cc and iqdmrg.cc which perform a DMRG ground-state calculation of the N=100 site S=1 (not $S = 1/2$!) Heisenberg chain. Although the codes are quite similar, note the use of quantum number conserving data types (IQMPS, IQMPO) in iqdmrg.cc.

Compile both codes using the commands "make dmrg" and "make iqdmrg". Run each and time them using the "time" command-line tool, for example "time ./dmrg".

A key advantage of using the quantum-number conserving code is the ability to obtain excited states that are the lowest energy state of their respective quantum-number sector. In the iqdmrg.cc code, edit the lines setting the "InitState" object "state" to flip a single spin from "Dn" to "Up". Increase the number of sweeps to at least 10. Recompile and run the iqdmrg code. Compute the energy difference between this excited state and the ground state. Do this again when you flip two spins. The first gap should be a very small number; the second should be about 0.4. The first gap is due to edge states on the ends of the chain; the second energy gap is the true bulk gap, first predicted by Haldane and known as the "Haldane gap".