Computational Methods in Many-Body Physics — Final Projects
Prof. M. Knap, Prof. F. Pollmann — Summer Term 2018
J. Hauschild — June 15, 2018

Projects marked with star are a bit more elaborate. Projects are assigned on a first come first serve basis.

Project 1: N-state Potts model (Monte Carlo)

Implement the Metropolis algorithm for the N-state Potts model in 2D and observe/discuss the behaviour of the phase transition for different N. The N-state Potts model is a generalization of the Ising model, where each s_i takes N possible values, and the Hamiltonian is given by $H = -J \sum_{\langle i,j \rangle} \delta_{s_i,s_j}$, where $\langle i, j\rangle$ denotes nearest neighbours and δ_{s_i,s_j} the Kronecker-delta.

Project 2: Criticality of the (classical) 3D Ising model (Monte Carlo)

Generalize the Swendsen-Wang algorithm to the (classical) Ising model on a 3D cubic lattice and perform a finite size scaling analysis to obtain the critical exponents.

Project 3*: The worm algorithm for the 6-vertex model (Monte Carlo)

Implement the worm algorithm for the 6-vertex model (`https://en.wikipedia.org/wiki/Ice-type_model`) at $T = \infty$ (where all allowed configurations are equally likely). Calculate the exponente a of the correlation function $\langle s_0 s_r\rangle \propto \frac{1}{r^a}$.

Project 4: Ground state properties of the 2D (transverse field) Ising model with Conservation laws (Exact Diagonalization)

Generalize (the code of) exercise 5 to the transverse field Ising model in 2 spatial dimensions, use both k_x and k_y as quantum numbers. Find the ground state (and possibly a few excited states) to locate the quantum phase transition.

Project 5: Krylov time evolution in a random Heisenberg chain (Exact Diagonalization)

In exercise 6 we used the Lanczos algorithm to find the ground state of H projected into the Krylov subspace and transformed it back to the full Hilbert space to find a good approximation of the ground state in the full Hilbert space. In a similar fashion, one can do a time evolution in the Krylov subspace to get an approximation of the time evolution in the full Hilbert space (`https://www.jstor.org/stable/2158085`). Use this method to perform the time evolution of a product state (e.g. $|\uparrow\downarrow\uparrow\downarrow\dots\rangle$) for the Heisenberg model with a random field, $H = J\sum_i \vec{S}_i \cdot \vec{S}_{i+1} - \sum_i h_i S_i^z$, where the values of the field $h_i \in [-W, W]$ are chosen from a uniform random distribution with a “disorder strength” W. Plot the growth of the entanglement entropy $S(t)$ for small $W = 0.5J$ and for large $W = 5J$.

Project 6: Construction of the reduced density matrix (MPS)

Use DMRG to calculate the ground state $|\psi\rangle$ of the transverse field Ising model for a large system ($L \approx 100$) as an MPS. Find a method to construct the reduced density matrix of n sites ($n \lesssim 10$) in the center. Measure the entanglement entropy of this subsystem of n sites for the different n.

Project 7*: Purification (MPS)

Purification (see e.g. the review by Schollwoeck) is a method to represent mixed states with MPS, which can be used to calculate thermodynamic properties from $\rho = e^{-\beta H}$. Calculate the energy, specific heat and magnetization as a function of temperature for the transverse field Ising model.

Project 8: Dynamical correlation functions (MPS)

Use the TEBD and DMRG to calculate correlation functions of the form $\langle\psi_0|\, e^{\mathrm{i}Ht} S_i^+ e^{-\mathrm{i}Ht} S_j^- \,|\psi_0\rangle$, where $|\psi_0\rangle$ is the ground state of the transverse field Ising model. Perform a fourier transformation in space and time and compare your results to the results of exercise 5.

Project 9*: DMRG for fermions (MPS)

Make use of the Jordan-Wigner transformation to write the Fermi-Hubbard Hamiltonain $H = -t\sum_{i,\sigma}(c^\dagger_{i,\sigma} c_{i+1,\sigma} + h.c.) - U\sum_i n_{i,\uparrow} n_{i,\downarrow}$ with fermionic creation operatos $c^\dagger_{i,\sigma}$ and $n_i = c^\dagger_i c_{i,\sigma}$ as an MPO. Use DMRG to find the ground state at half filling (i.e. for $N = L$ particles, where L is the number of sites, $i = 0, \ldots L-1$) and calculate correlation functions $\langle c^\dagger_{i\sigma} c_{j\tilde{\sigma}}\rangle$ for different interaction strengths U. Some explanations: `https://tenpy.github.io/intro_JordanWigner.html`.

Project 10: Phase diagram of the 1D Bose-Hubbard model (MPS)

Use DMRG to find the ground states of the interacting 1D Bose-Hubbard model $H = -t\sum_i(a^\dagger_i a_{i+1} + h.c.) + \frac{U}{2}\sum_i n_i(n_i - 1) - \mu\sum_i n_i$ for different choices of the parameters t, U, μ. Note that you need to cut off the maximum number of bosons on each site to $n_c = 1, 2, 3, \ldots$. Calculate the correlation function of superfluid order $\langle a^\dagger_i a_{i+r}\rangle$ and the density $\langle n_i\rangle$ and use them to determine the ground state phase diagram. Compare the influence of different cutoffs n_c on the result.

Project 11: Correlations and entanglement in the Heisenberg critical point (MPS)

Use DMRG to find the ground state of the Heisenberg model $H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$. Calculate spin-spin correlations. Use the scaling of the half-chain entanglement entropy with system size L to extract the central charge c from $S(L) = \frac{c}{6} \log(L)$ valid for large L.

Project 12: Heisenberg model with short and exponential decaying interactions (MPS)

There is a natural way to write down matrix product operators for interactions which decay exponentially in distance, here we consider $H = \sum_i \sum_{j>i} J e^{-\frac{|i-j|}{\xi}} \vec{S}_i \cdot \vec{S}_j$. Use DMRG to find the ground state. Find out which influence ξ has on the correlations $\langle S_i^z S_j^z \rangle$.

Project 13*: Stochastic Series Expansion for a bond alternating Heisenberg model (Quantum Monte Carlo)

Generalize the code of the stochastic series expansion of the Heisenberg model to work with couplings strength J and J' for different bonds, of the pattern shown in the figure to the right. Calculate the energy, specific heat and staggered magnetization as a function of temperature for different values of $0 \leq J' \leq 1$ and fixed $J \equiv 1$.