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Computational Many-Body Physics

Exercise Sheet 4

Summer Term 2024

Due date: Wednesday, **12th June** 2024

Website: thp.uni-koeln.de/trebst/Lectures/2024-CompManyBody.shtml

This week's sheet is devoted to **quantum Monte Carlo** techniques. We will guide you through an implementation of the stochastic series expansion and use it to study a thermal phase transition in a quantum spin model.

Exercise 8: Stochastic Series Expansion

We start by looking for footprints of a thermal phase transition in the quantum spin-$\frac{1}{2}$ Heisenberg model on the cubic lattice, which is described by the Hamiltonian

$$H = -J \sum_{\langle i,j\rangle,\gamma} \hat{S}_i^\gamma \hat{S}_j^\gamma = -J \sum_{\langle i,j\rangle} \left(\hat{S}_i^z \hat{S}_j^z + \hat{S}_i^y \hat{S}_j^y + \hat{S}_i^x \hat{S}_j^x \right) , \tag{1}$$

where the spin operators $\hat{S}_i^\gamma$ now refer to Pauli matrices. We set the coupling constant to $J = -1$ for antiferromagnetic interactions and sum runs over all pairs of nearest neighbors of the lattice.
To study this model we want using quantum Monte Carlo simulations ased on the stochastic series expansion (SSE). At its heart, SSE is based on rewriting the Boltzmann factor in the partition function as a Taylor expansion [1]

$$Z = \mathrm{Tr} e^{-\beta H} = \sum_\alpha \sum_{n=0}^{\infty} \left\langle \alpha \left| \frac{(-\beta H)^n}{n!} \right| \alpha \right\rangle . \tag{2}$$

It is particularly useful to rewrite the Hamiltonian in terms of contributions of every bond

$$H = -\sum_b H_b \tag{3}$$

$$= -\sum_b \left[\underbrace{\left(\hat{S}_{b_1}^z \hat{S}_{b_2}^z - \frac{1}{4} \right)}_{\text{diagonal}} + \underbrace{\frac{1}{2} \left(\hat{S}_{b_1}^+ \hat{S}_{b_2}^- + \hat{S}_{b_1}^- \hat{S}_{b_2}^+ \right)}_{\text{off-diagonal}} \right] + const. \tag{4}$$

The constant absorbs the shift of the Hamiltonian induced by the artificially introduced addition of $\frac{1}{4}$ per bond. This form of the Hamiltonian is perfectly adapted to the needs of SSE, namely that all non-zero matrix elements ($\langle\uparrow\uparrow |H_b| \uparrow\uparrow\rangle, \langle\downarrow\downarrow |H_b| \downarrow\downarrow\rangle, \langle\uparrow\downarrow |H_b| \downarrow\uparrow\rangle, \langle\downarrow\uparrow |H_b| \uparrow\downarrow\rangle$) have the same value of $\frac{1}{2}$ in this case.
The first part of the exercise will focus on implementing the SSE algorithm. For this we will

[1] A good reference for an introduction to SSE is this book chapter by Anders Sandvik at arXiv:1909.10591.

divide its implementation into multiple parts, separately discussing diagonal and off-diagonal updates.

a) To set the stage, you need to implement a **cubic lattice** and all the necessary data structures. For starters, you need an array containing all the spin information of the lattice and an array for all applied operators. What size does the operator array need to be? Since we will loop over all nearest bonds of the lattice, you need to define them (note that you might want to implement periodic boundary conditions).

b) In the **diagonal update** part of the simulation, diagonal operators are added/removed with a probability p_{add}/p_{rem}. How are the probabilities defined? There are no constraints on removing a diagonal operator, while inserting it is allowed only if the bond spins are antiparallel. Encountering an off-diagonal operator will cause the spin states at the bond to flip. Implement a function for the diagonal updates. To test your function, apply it repeatedly to an initial spin state and count the number of diagonal operators at the end. Repeat this process for different temperatures and create a histogram of the operator count.

c) The **off-diagonal updates** always involve updating at least *two* operators. To perform the updates efficiently, we will implement a loop update algorithm. For the loop construction, it is useful to introduce another data structure in which the *connectivity* of the operators is explicitly represented. This *vertex* structure is a spin operator object that contains information about the operator and the connected spins Fig. [1].
The vertices are connected by the operators applied to the mutual spins. This is best done by keeping a list that assigns an index of the connected vertex to each vertex. This list can then be updated by iterating over each vertex and checking for a connection.Ẇrite a linkvertex() function and apply it to a random spin/operator configuration. Check that the resulting vertex loops are closed.

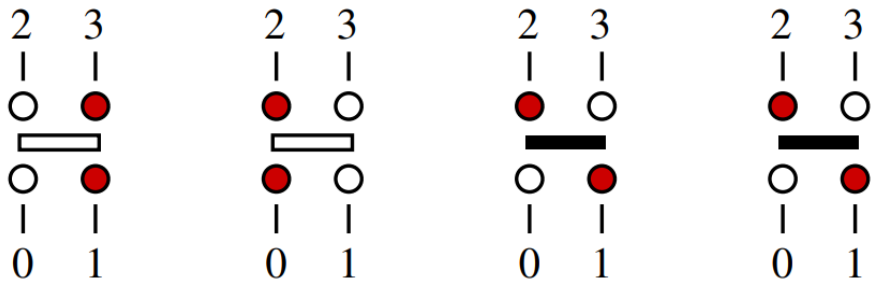

Figure 1: The different **allowed vertices**. The red/white represent the spins in the ± 1 state and white/black bars represent the diagonal/off-diagonal operators. The numbering of the spins corresponds to the state of the connected spins before and after the operator acts.

d) Now we only need to perform the off-diagonal update, by flipping the **vertex loops** with a probability of $1/2$. Flipping the loops will change the involved operators from diagonal to off-diagonal operators and vice versa, additionally all spins not connected to any operator are flipped.

In order to run the full simulations, you now need to put the different parts together. A single sweep of the simulation is done by performing the diagonal update, creating the vertices loop and performing the loop updates.
In general, we would have to determine the maximum expansion order Λ – a step which is

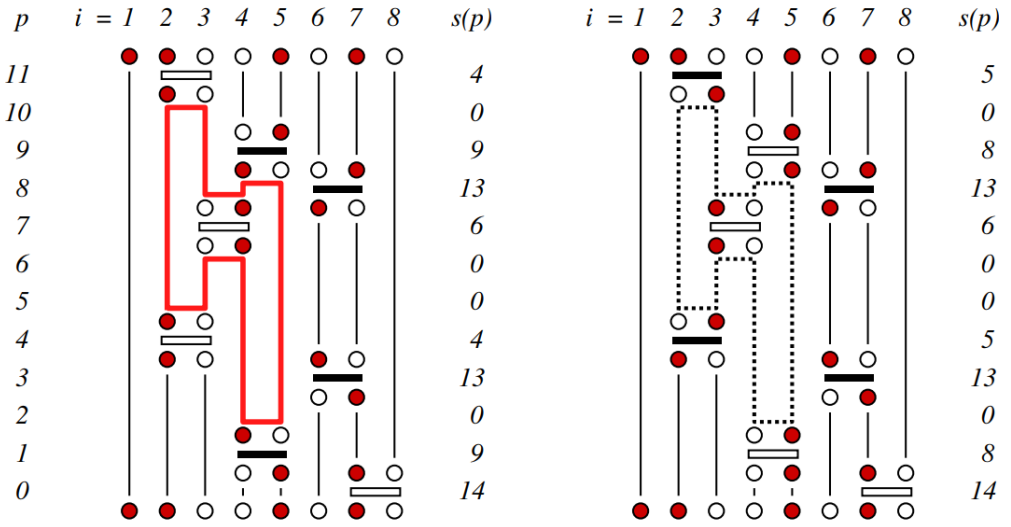

Figure 2: **A linked-vertex SSE configuration**. The left side shows a constructed loop of connected vertices before flipping it and the right side shows the configuration after flipping the loop. All spin orientations are flipped and the operators are changed from diagonal to off-diagonal and vice versa.

typically done during a thermalization run. Here we will simply fix it to $\Lambda = 2\beta L^3$.

e) Perform simulations for inverse temperatures $\beta = 0.2, 0.4, 0.6, \ldots 5.0$ and varying system sizes $L = 8, 12, 16$. Measure the **staggered magnetization** m_s and plot $m_s L^3/(L^{(2-0.034)})$ against the inverse temperature β. The staggered magnetization is calculated by spatially alternating the sign of spins. For example, in a 2 by 2 square lattice the staggered magnetization would be $m_s = \pm(S_{11} - S_{12} - S_{21} + S_{22})$. It should be sufficient to do 10^4 measurement steps (sweeps) after a considerable thermalization time (usually 10% of the number of sweeps).

f) Remember that the **energy** can be elegantly obtained by simply measuring the expansion order n as $\langle E \rangle = -\frac{\langle n \rangle}{\beta}$. Plot the energy per spin against the inverse temperature β. What observable can you deduce from the energy that will allow you to clearly identify signatures of the thermal phase transition?

Similar to the lecture video, you might also want to plot the **average expansion order** $\langle n \rangle$ or, even better, a histogram of the sampled expansion orders as a function of the inverse temperature.