Quantum Monte Carlo - Heisenberg spin chain

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A short Monte Carlo program for simulating the 1D ferromagnetic Heisenberg spin chain.

1 Theory

We are dealing with a 1d ferromagnetic quantum spin chain with periodic boundary conditions and nearest neighbour coupling. The Hamiltonian is:

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \vec{S}_j, \tag{1}$$

and the partition fucntion:

$$Z(\beta) = \operatorname{tr} \exp(-\beta H) = \sum_{b_1} \langle b_1 | \exp(-\beta H) | b_1 \rangle \tag{2}$$

The interaction is split to even and odd terms which commute:

$$H = A + B = -\frac{J}{4} \left(\sum_{k=1}^{n/2} \vec{\sigma}_{2k-1} \cdot \vec{\sigma}_{2k} + \sum_{k=1}^{n/2} \vec{\sigma}_{2k} \cdot \vec{\sigma}_{2k+1} \right) \tag{3}$$

Using the Trotter-Suzuki decomposition:

$$\exp(z(A+B)) = \exp(\frac{z}{n}(A+B))^n = (\exp(\frac{z}{n}A) \exp(\frac{z}{n}B))^n + \mathcal{O}(\frac{z^2}{n}) \tag{4}$$

we split the exponent into $\frac{M}{2}$ terms. Inserting $M-1$ identities $\sum_b |b\rangle\langle b|$ we get the partition function with $z = \frac{J}{4}(2\beta/M)$:

$$Z(\beta) = \sum_{b_1, b_2, \ldots, b_M} \langle b_1 | \exp(zA) | b_2 \rangle \langle b_2 | \exp(zB) | b_3 \rangle \ldots \langle b_M | \exp(zB) | b_1 \rangle. \tag{5}$$

As terms in exponents A and B commute, the partition function can be written using the matrix elements of a two particle operator:

$$U^{(2)}(z) = \exp(z \vec{\sigma}_1 \cdot \vec{\sigma}_2), \tag{6}$$

with six non zero matrix elements:

$$\begin{aligned} W(a) &= \langle 11 | \exp(z \vec{\sigma}_1 \cdot \vec{\sigma}_2) | 11 \rangle = \langle 00 | \exp(z \vec{\sigma}_1 \cdot \vec{\sigma}_2) | 00 \rangle = e^z \\ W(b) &= \langle 10 | \exp(z \vec{\sigma}_1 \cdot \vec{\sigma}_2) | 01 \rangle = \langle 01 | \exp(z \vec{\sigma}_1 \cdot \vec{\sigma}_2) | 10 \rangle = e^{-z} \sinh(2z) \\ W(c) &= \langle 10 | \exp(z \vec{\sigma}_1 \cdot \vec{\sigma}_2) | 10 \rangle = \langle 01 | \exp(z \vec{\sigma}_1 \cdot \vec{\sigma}_2) | 01 \rangle = e^{-z} \cosh(2z) \end{aligned} \tag{7}$$

Sampling for the spin chain of length n will be done on a $n \times M$ lattice of classical spins. As H is a product of even and odd two particle operators, the spins have to be oriented appropriately, otherwise we get a zero. An example of valid configurations is shown on 1.

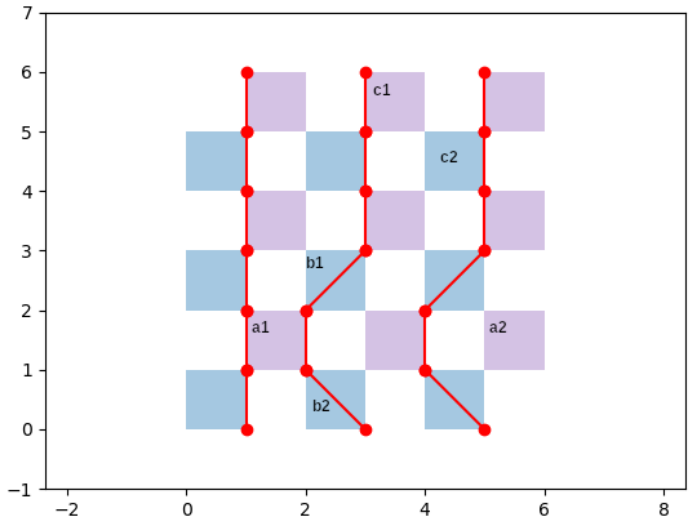

Figure 1: Blue tiles depict the application of a two particle operator on even time slices and the purple ones are odd. Valid local tiles are shown (a1, a2, b1, b2, c1, c2).

To get the statisical weight of a state, we loop over the lattice and multiply the weights of tiles 7. The boundary condition is periodic in the spatial and time direction.

2 Algorithm

A type of loop algorithm is used similar to the Swendsen Wang algorithm.

1. Make bonds between spins on a tile.
2. Find loops.
3. Flip the spins in each loop with probability $\frac{1}{2}$.
4. Perform measurements.

Depending on the tile type, different types of bonds between spins are possible.

To satisfy the detailed balance condition we need to determine the bond forming probabilities. Tile types b and c have only one posssible bond type.

$$P(b \to a) = P(c \to a) = 1/2 \tag{8}$$

For tile type a, we need to determine the probability for each bond type.

$$\begin{aligned} W(a)P(a \to b) = W(a)P(a,\times)/2 = W(b)P(b \to a) = W(b)/2 \\ W(a)P(a \to c) = W(a)P(a,||)/2 = W(c)P(c \to a) = W(c)/2 \end{aligned} \tag{9}$$

From which it follows:

$$\begin{aligned} P(a,\times) &= W(b)/W(a) \\ P(a,||) &= W(c)/W(a) \\ P(a,||) + P(a,\times) &= 1. \end{aligned} \tag{10}$$

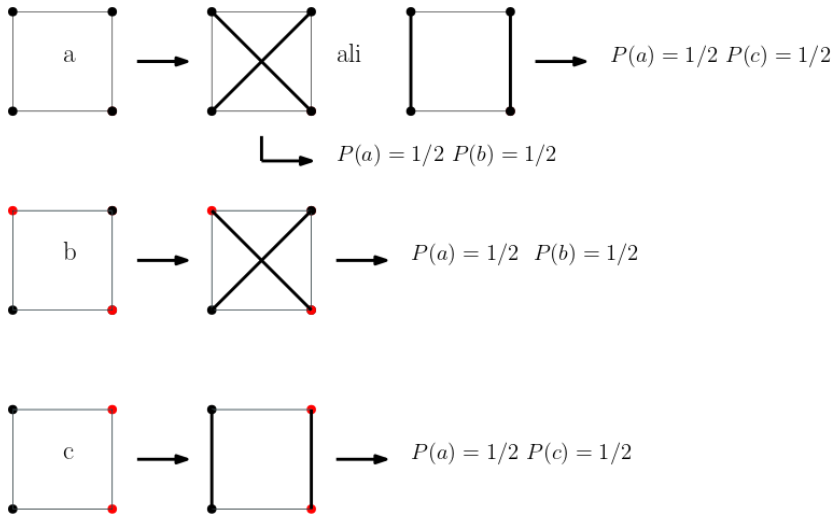

Figure 2: Possible bonds for each tile type. Probabilities for each tile type after a random spin flip are also shown.

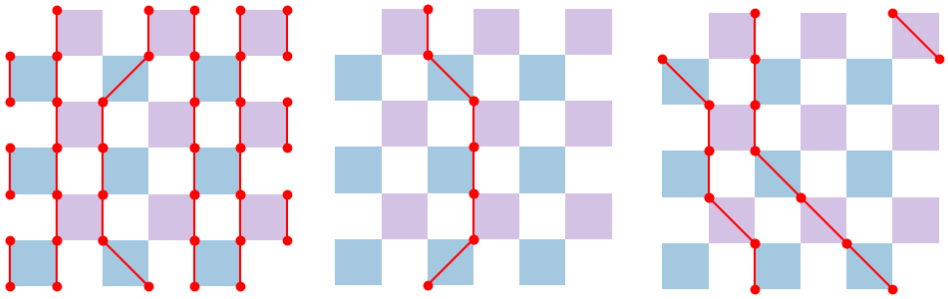

Figure 3: Configurations in consecutive updates.

We did not take into account that spins on a given tile can be a part of the same loop because of the periodic boundaries, but the probability for this to happen is not dependent on the tile type and it does not break the detailed balance condition.

Diagonal observables are simple to calculate:

$$\mathcal{O} = \frac{\operatorname{tr}\exp(-\beta H)\mathcal{O}}{\operatorname{tr}\exp(-\beta H)} = \frac{\sum_{b_1,b_2,\ldots,b_M}\langle b_1|\mathcal{O}|b_1\rangle\langle b_1|\exp(zA)|b_2\rangle\langle b_2|\exp(zB)|b_3\rangle\ldots\langle b_M|\exp(zB)|b_1\rangle}{\sum_{b_1,b_2,\ldots,b_M}\langle b_1|\exp(zA)|b_2\rangle\langle b_2|\exp(zB)|b_3\rangle\ldots\langle b_M|\exp(zB)|b_1\rangle}. \tag{11}$$

To calculate the energy we use the known relation:

$$\langle H\rangle = -\frac{\mathrm{d}}{\mathrm{d}\beta}\log(Z(\beta)). \tag{12}$$

3 Results

Results are shown for spin chains of length $n = 4, 6, 12$ and compared to results from a direct diagonalization.

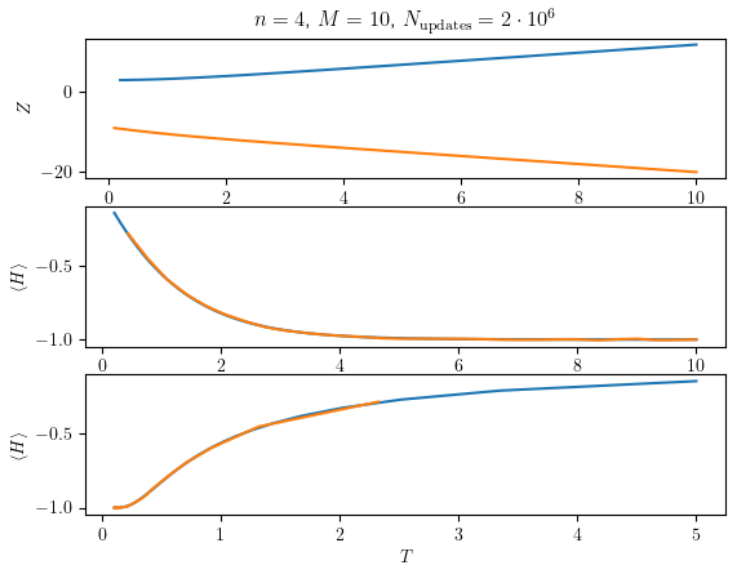

Figure 4: The partition function as a function of the inverse temperature for $n = 4$ spin chain and the energy.

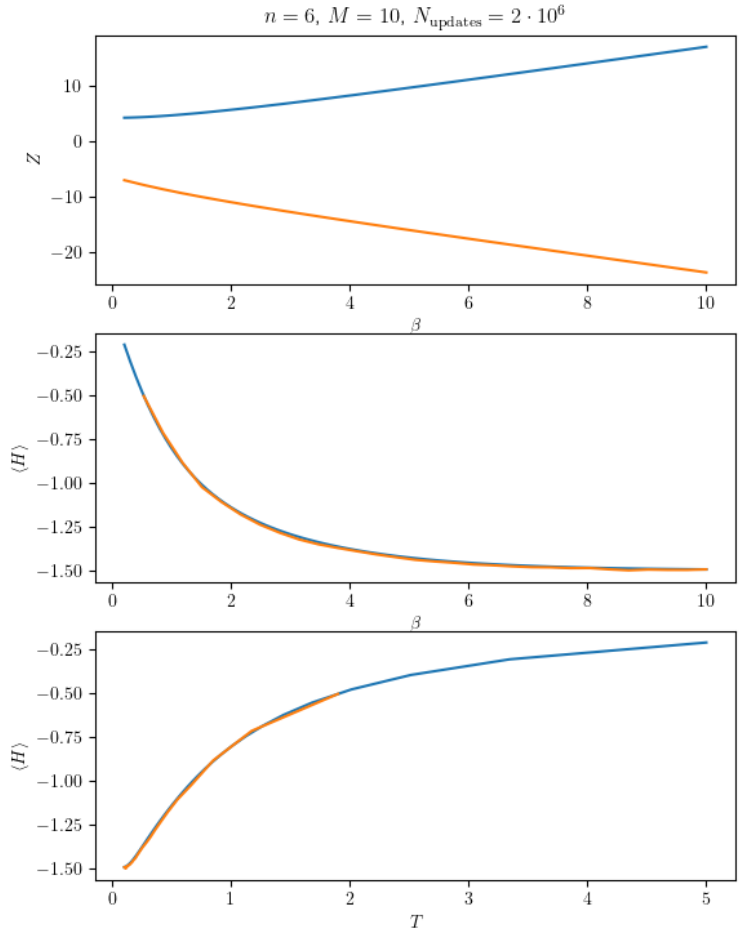

Figure 5: The partition function as a function of the inverse temperature for $n = 6$ spin chain and the energy.

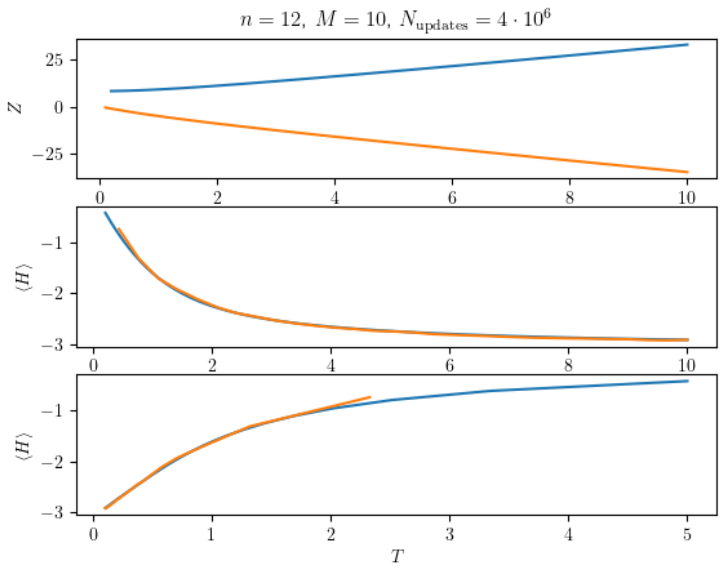

Figure 6: The partition function as a function of the inverse temperature for $n = 12$ spin chain and the energy.