FYS4150: Project 4

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1 Introduction

The aim of this project is to study the Ising model in two dimensions.

2 The Ising model (ch. 13)

The Ising model describes pahse transitions in two dimensions. At a given critical temperature the model exhibits a phase transition from one magnetic moment (spin) to a phase with zero magnetization. Without an externally applied field, this is described as

$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{1}$$

where $s_k = \pm 1$, N is the total number of spins and J is a coupling constant.

3 The Metropolis algorithm (ch. 12)

4 2x2 lattice

We consider a 2×2-lattice, meaning $L = 2$. The spins have 16 conifgurations. The probability distribution is given by

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{2}$$

where $\beta = \frac{1}{kT}$ is the inverse temperature, k is te Boltzmann constant, E_i is the energy of a state i. The partition function is

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{3}$$

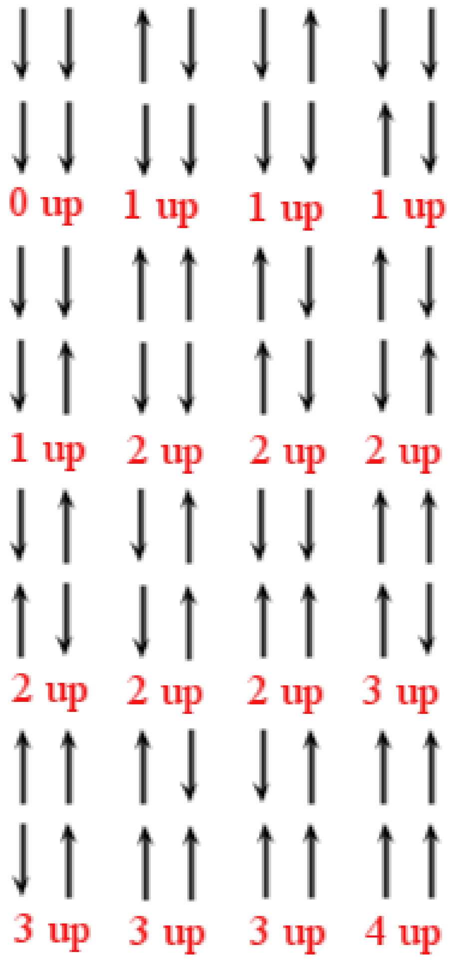
This fuction is difficult to compute since we need all states. The Metropolis algorithm only considers *ratios* between probabilities, so we don't need to calculate this (luckily!)

$$\text{Metropolis } \rightarrow \frac{P_s}{P_t} = \frac{e^{-(\beta E_s)}}{e^{-(\beta E_k)}} = e^{-\beta(E_s - E_k)} = e^{-\beta \Delta E}$$

The partition function in our case is

$$\begin{aligned} Z(\beta) &= \sum_{i=1}^{M} e^{-(\beta E_i)} \\ &= 2e^{8J\beta} + 2e^{-8J\beta} + 12 \\ &= 4(3 + \cosh(8J\beta)) \end{aligned}$$

The energy expectation value



(a) Different spin configurations

№of spins pointing up	Degeneracy	E	M
0	1	-8J	-4
1	4	0	-2
2	4	0	0
2	2	8J	0
3	4	0	2
4	1	-8J	4

(b) Possible energies for a 2×2-lattice of spin particles.

Figure 1: Spins for a 2×2-lattice with periodic boundary conditions.

$$\begin{aligned}
\langle E \rangle &= -\frac{\partial \ln Z}{\partial \beta} = -\frac{\partial \ln Z}{\partial Z}\frac{\partial Z}{\partial \beta} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} \\
&= -\frac{4 \cdot 8J \sinh(8J\beta)}{4(3+\cosh(8J\beta))} \\
&= -8J\frac{\sinh(8J\beta)}{3+\cosh(8J\beta)}
\end{aligned}$$

with the corresponding variance

$$\begin{aligned}
\sigma^2 = \langle E^2 \rangle - \langle E \rangle^2 &= \frac{1}{Z}\sum_{i=1}^{M} E_i^2 e^{-\beta E_i} - \Big(\frac{1}{Z}\sum_{i=1}^{M} E_i e^{-\beta E_i}\Big)^2 \\
&= \frac{8^2J^2 2e^{8J\beta} + 8^2J^2 2e^{-8J\beta} + 0 \cdot 12}{4(3+\cosh(8J\beta))} - \Big(-8J\frac{\sinh(8J\beta)}{3+\cosh(8J\beta)}\Big)^2 \\
&= 32J^2\frac{2\cosh(8J\beta)}{(3+\cosh(8J\beta))} - 64J^2\frac{\sinh^2(8J\beta)}{(3+\cosh(8J\beta))^2} \\
&= J^2 64\frac{\cosh(8J\beta)(3+\cosh(8J\beta)) - \sinh^2(8J\beta)}{(3+\cosh(8J\beta))^2} \\
&= J^2 64\frac{3\cosh(8J\beta) + \cosh^2(8J\beta) - \sinh^2(8J\beta)}{(3+\cosh(8J\beta))^2} \\
&= J^2 64\frac{3\cosh(8J\beta)+1}{(3+\cosh(8J\beta))^2}
\end{aligned}$$

The specific heat capacity

$$C_V = \frac{1}{k_B T^2}(\langle E^2 \rangle - \langle E \rangle^2) \tag{4}$$

$$C_V = \frac{64J^2}{k_B T^2}\frac{3\cosh(8J\beta)+1}{(3+\cosh(8J\beta))^2}$$

The mean absolute value of the magnetic moment (mean magnetization)

$$\begin{aligned}
\langle|\mathcal{M}|\rangle &= \frac{1}{Z}\sum_i^M |\mathcal{M}_i| e^{-\beta E_i} \\
&= \frac{1}{4(3+\cosh(8J\beta))}(4e^{8J\beta} + 4\cdot 2e^0 + 2\cdot 4e^0 + 4e^{8J\beta}) \\
&= 2\frac{e^{8J\beta}+2}{3+\cosh(8J\beta)}
\end{aligned}$$

The susceptibility

$$\chi = \frac{1}{k_B T}(\langle\mathcal{M}^2\rangle - \langle\mathcal{M}\rangle^2) \tag{5}$$

$$\begin{aligned}
\chi &= \frac{1}{k_B T}(\frac{1}{Z}\sum_i^M \mathcal{M}_i^2 e^{-\beta E_i} - \Big(\frac{1}{Z}\sum_i^M \mathcal{M}_i e^{-\beta E_i}\Big)^2) \\
&= \frac{1}{k_B T}\frac{(16e^{8J\beta} + 4\cdot 4e^0 + 4\cdot 4e^0 + 16e^{8J\beta})}{4(3+\cosh(8J\beta))} \\
&= \frac{1}{k_B T}\frac{8e^{8J\beta}+8}{(3+\cosh(8J\beta))}
\end{aligned}$$

The analytical values (calculated in Python) are found in table (**??**).

Z	$\langle E\rangle$	$\langle\lvert\mathcal{M}\rvert\rangle$	C_V	χ
5973.917	-7.9839	3.9946	0.1283	15.9732

Figure 2: Analytical values of the expectation values. Here $J = 1$, $k = 1$, $T = 1.0$ K.

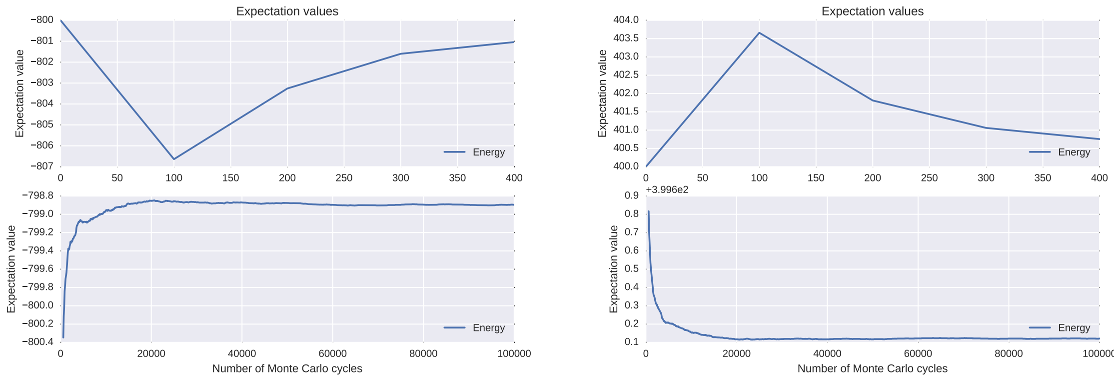
For $mcs = 1000000$ cycles the results are very similar to the analytic results.

5 20x20 lattice

Setting temperature to $T = 1$ and running a 20×20 lattice for a different number of Monte Carlo cycles ranging from 1 to 10^{-7}. We see from figure (3) that for 1 cycle energy and magnetization are exactly -800 and 400. This is because when one random spin is flipped the probability of keeping this energy configuration is proportional to $e^{-8} \simeq 0.0003$. As we add more cycles, however, the probability of some spins using their new configuration becomes larger. Both expectation values seem to stabilize at around 10^5.

We also look at a system that begins with a random distribution of spins. For a 20×20-lattice this will probably begin with energy 0 and magnetization 0. It will the 'tip' to one of the sides, and converge towards -800 and 400. The results are shown in fig (4).

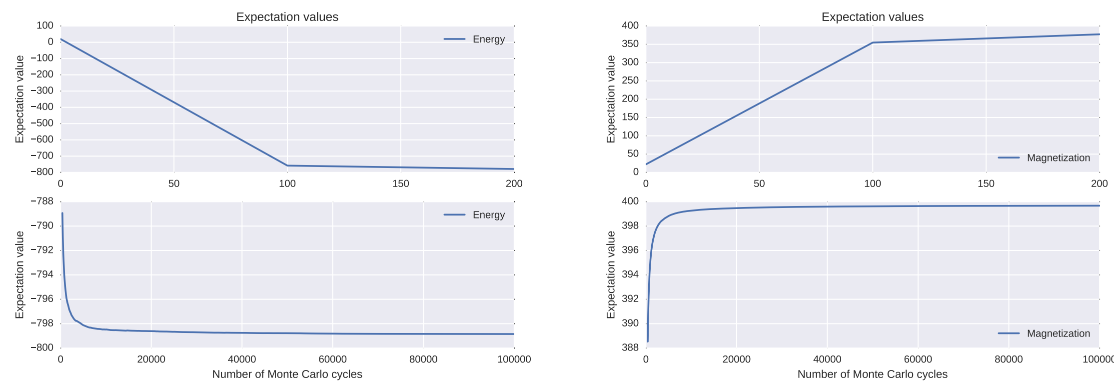
We also run the program for temperature $T = 2.4$. The stable energy and magnetization are now smaller in norm.



(a) Expectation value energy.

(b) Expectation value magnetization.

Figure 3: 20×20-lattice with temperature $T = 1$, ordered initial configuration.



(a) Expectation value energy.

(b) Expectation value magnetization.

Figure 4: 20×20-lattice with temperature $T = 1$, random initial configuration. Used 10000 points.

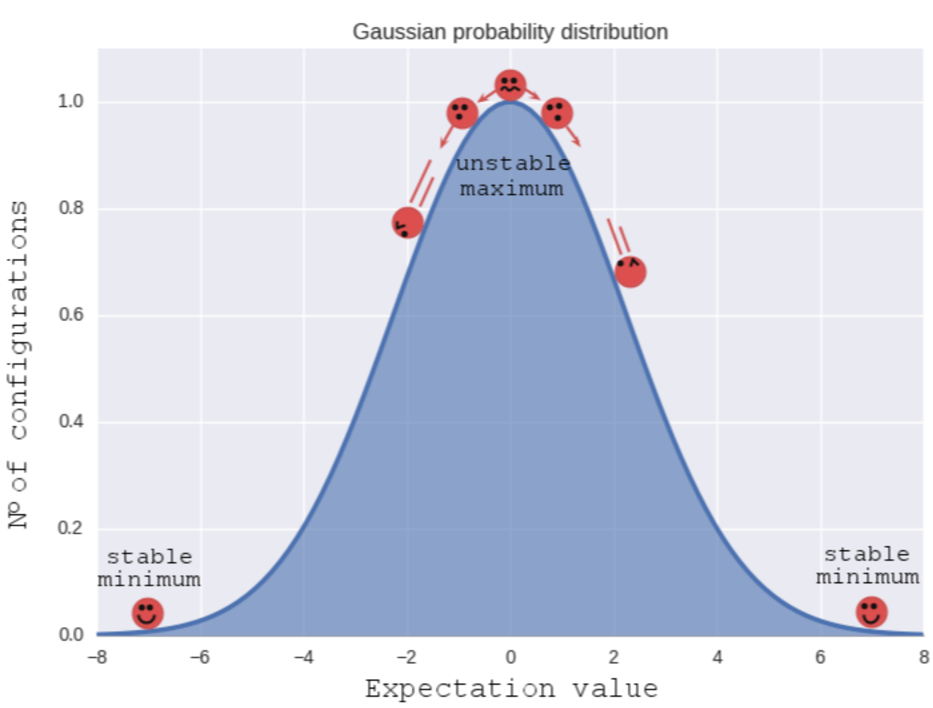
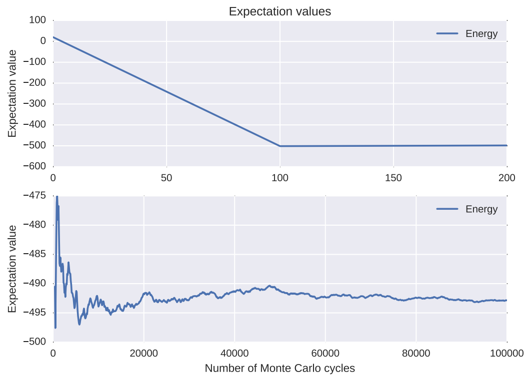
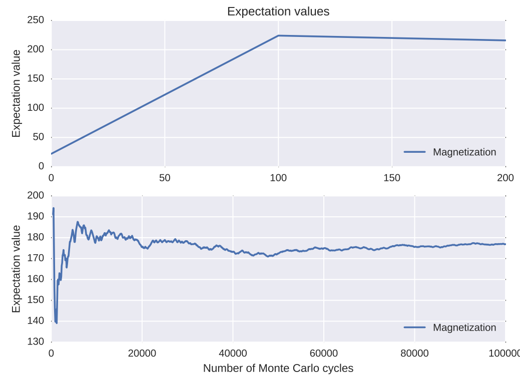


Figure 5: Expectation configuration distribution

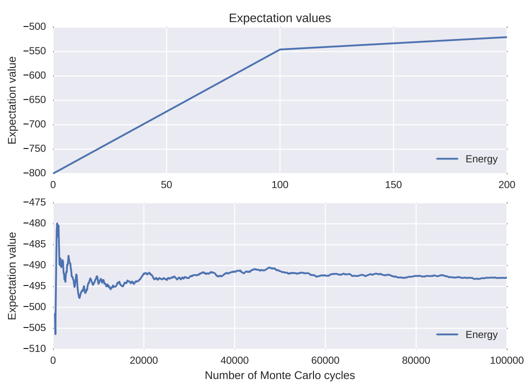


(a) Expectation value energy.

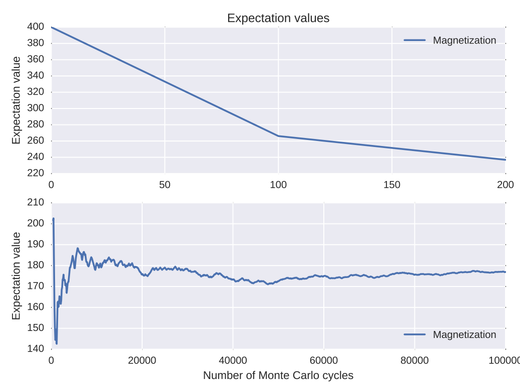


(b) Expectation value magnetization.

Figure 6: 20×20-lattice with temperature $T = 2.4$, random initial configuration. Used 10000 points.

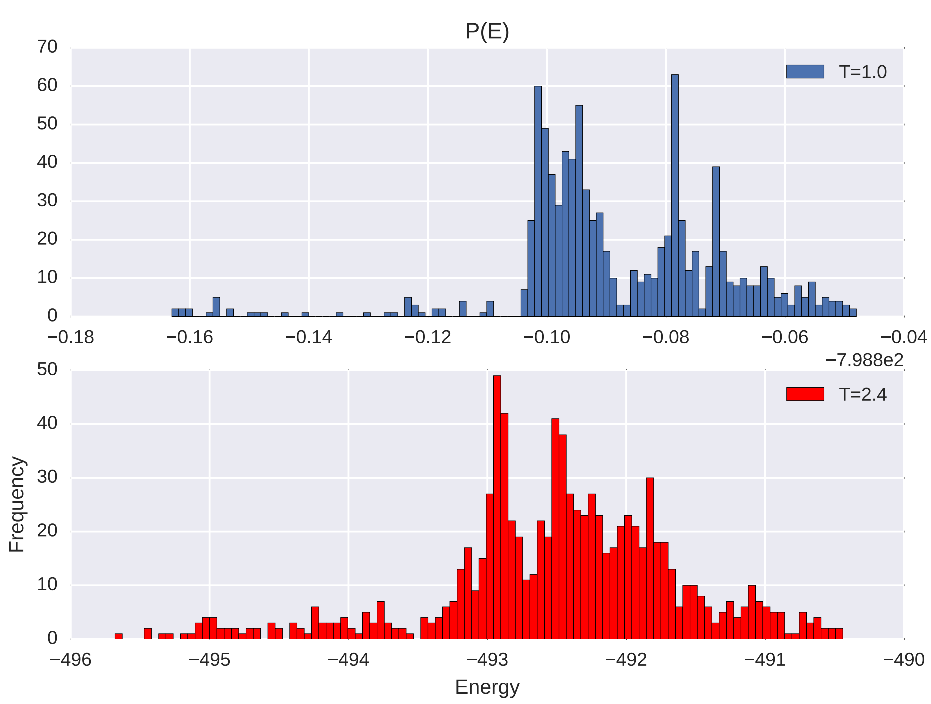


(a) Expectation value energy.



(b) Expectation value magnetization.

Figure 7: 20×20-lattice with temperature $T = 2.4$, ordered initial configuration. Used 10000 points.



6 Analyzing the probability distribution

We find the probability of a state by counting the number of states in an energy E, and dividing by the total number of configurations

$$P(E) = \frac{N(E)}{cms} \tag{6}$$

where cms is the number of Monte Carlo cycles used. We see from the results in Fig. (**??**) that the probability distribution is much narrower for $T = 1.1$.
After running 10^5 monte carlo cycles, the variance is for $1T$: $\sigma_E = -3.58476$, for $T = 2.4$: $\sigma_E = 3161.7$.

7 Sources