Computer simulation in pysics

Interacting spins in a heat bath

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1 Motivation

When I leaned to the quantum mechanics exam, I made a small detour at dawn of the internet and I saw a visualisation about the Ising spin model. This visualisation was the key to understand this problem. Because of this I decided to try to simulate this system.

2 Abstract

The master equation for two ferromagnetically coupled Ising spins is considered. The system is assumed to be in contact with a heat bath at temperature T . Accordingly, the transition rates in master-equation are chosen so that the system relaxes to equilibrium at temperature T . The solution of the master equation is derived and the relaxation of the magnetization of the system is obtained.

Step of the simulation:

- We randomly select a spin.
- Let's see how much we change the energy of the system if we rotate it.
- If $\Delta < 0$, we rotate the spin and go to point *(1)*.
- If $\Delta = 0$ then we take a random number P from the interval *[0, 1]*and if P < *1/2*, we rotate the spin and go to point *(1)*. If P > *1/2*, we go to point *(1)* without rotation
- If $\Delta > 0$, we take a random number P from the interval *[0, 1]*, and if $P < e^{(-\beta\Delta E)}$, we rotate the spin, otherwise we go to point *(1)*.

Spins interact ferromagnetically with their neighbors, so the energy of a state is as follows:

$$E(s_1, s_2 ...., s_N) = J \sum_{1}^{N-1} s_i s_{i+1}, \quad J > 0. \tag{2.1}$$

Spins interact with a T-temperature environment and, as a result, can flip from one state to another. Choose a shape for the spin-flip rate that satisfies the principle of detailed balance. This will be the case, for example, if the i-th spin rotation rate in the following (1 / s unit):

$$w(s_1, ..., s_{i-1}, s_i, s_{i+1, ... s_N}) = \begin{cases} 1 & ha \;\; \Delta E < 0 \\ 1/2 & ha \;\; \Delta E = 0 \\ e^{(-\beta\Delta E)} & ha \;\; \Delta E > 0 \end{cases} \tag{2.2}$$

where as easy to see:

$$\Delta E = 2Js_i(s_{i-1} + s_{i+1}). \tag{2.3}$$

I am trying to determine $\langle m \rangle$ and the $\langle m^2 \rangle$ averages with some βJ values at appropriate temperatures.
In the simulation we have four different N and take 15pc βJ number randomly, where $J = 1$.

3 Introduction and theoretical background

For the understand of the theoretical background the system consists of two Ising spins, s_1 and s_2, the spins can take two values $s_i = \pm 1$. The ferromagnetic interaction between the two spins described by:

$$E(s_1, s_2) = -Js_1 s_2, \tag{3.1}$$

where J is a positive constant. The spins are in contact with a heat bath of temperature T and after a long time the spins will be in equilibrium a T, which means that the probability of a state (s_1, s_2) is given by:

$$P^e(s_1, s_2) = \frac{1}{Z} e^{-\beta E(s_1, s_2)} = \frac{1}{Z} e^{\beta J_{s_1, s_2}}, \tag{3.2}$$

where $\beta = \frac{1}{k_B T}$ and Z is the partition function obtained from the condition:

$$\sum_{s_1=\pm 1} \sum_{s_2=\pm 1} P^{(e)}(s_1, s_2) = \frac{1}{Z} \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} e^{\beta J_{s_1 s_2}} = 1. \tag{3.3}$$

If we introducing $K = \beta J$,

$$Z = 2(e^{2K} + e^{-2K}) \tag{3.4}$$

and we put this in 3.2. equation, we cab get the equilibrium distribution:

$$P^{(e)}(s_1, s_2) = \frac{e^{K_{s_1 s_2}}}{2(e^{2K} + e^{-2K})} \tag{3.5}$$

We got two high-energy states $E(\downarrow\uparrow) = E(\uparrow\downarrow) = J$ and two low-energy $E(\uparrow\uparrow) = E(\downarrow\downarrow) = -J$, and the corresponding equilibrium probabilities are as follows

$$P^{(e)}(\uparrow\uparrow) = P^{(e)}(\downarrow\downarrow) = \frac{e^K}{Z}, \tag{3.6}$$
$$P^{(e)}(\uparrow\downarrow) = P^{(e)}(\downarrow\uparrow) = \frac{e^{-K}}{Z} \tag{3.7}$$

For the introduce dynamics we have to use the master-equation for the time-dependent. This one is the nonequilibrium distribution,

$$\frac{\partial P(s_1, s_2; t)}{\partial t} = -[w_1(s_1, s_2) + w_2(s_1, s_2)]P(s_1, s_2; t) + \tag{3.8}$$
$$+w_1(-s_1, s_2)P(-s_1, s_2; t) + w_2(s_1, -s_2)P(s_1, -s_2; t), \tag{3.9}$$

where the w the rate of the flips. But we need a system which relaxes to equilibrium. Since the detailed balance should be satisfied in equilibrium, we have the following conditions for the flip rates:

$$w_1(s_1, s_2)P^{(e)}(s_1, s_2) = w_1(-s_1, s_2)P^{(e)}(-s_1, s_2) \tag{3.10}$$
$$w_2(s_1, s_2)P^{(e)}(s_1, s_2) = w_2(s_1, -s_2)P^{(e)}(s_1, -s_2) \tag{3.11}$$

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If we use the 3.5. equation we got:

$$w_1(\uparrow\uparrow) = w_2(\uparrow\uparrow) = w_1(\downarrow\downarrow) = w_2(\downarrow\downarrow) = e^{-2K} \tag{3.12}$$
$$w_1(\uparrow\downarrow) = w_2(\uparrow\downarrow) = w_1(\downarrow\uparrow) = w_2(\downarrow\uparrow) = 1 \tag{3.13}$$

The above flip rates are frequently used. They correspond to the choice of rates of $w = 1$ if the flip decreases the energy while $w = e^{-\beta\delta E}$ if the flip increases the energy ($\delta E > 0$).

If we use the 3.12 and 3.13. equation and write the master equation in a matrix form,

$$\partial\vec{P}(t) = \mathbf{A}\vec{P}(t), \tag{3.14}$$

where $\mathbf{A}$ is called evolution matrix,

$$\mathbf{A} = \begin{bmatrix} -2e^{-2K} & 1 & 1 & 0 \\ e^{-2K} & -2 & 0 & e^{-2K} \\ e^{-2K} & 0 & -2 & e^{-2K} \\ 0 & 1 & 1 & -2e^{-2K} \end{bmatrix} \tag{3.15}$$

The equilibrium distribution is a stationary solution of the master equation which means that the vector

$$\vec{P}^{(e)} = \frac{1}{2(e^{K}+e^{-K})} \cdot \begin{bmatrix} e^{K} \\ e^{-K} \\ e^{-K} \\ e^{K} \end{bmatrix} \tag{3.16}$$

is an eigenvector of the matrix $\mathbf{A}$ with eigenvalue $\lambda_1 = 0$. This can be easily verified by just calculating $\mathbf{A}\vec{P}^{(e)}$.

$$\vec{P}^{i}(t) = a_i e^{\lambda_i t}\vec{P}_i \tag{3.17}$$

where $\vec{P}^{(i)}(0) = a_i\vec{P}^{(i)}$. All the eigenvectors of the matrix $\mathbf{A}$ are symmetric. The four algebraic equations obtained from the components of the eigenvalue equation

$$\mathbf{A}\vec{P}^{(i)} = \lambda_i\vec{P}^{(i)} \tag{3.18}$$

are not independent. They yield only two equations

$$-2e^{-2K}\cdot a + 2b = \lambda_i \cdot a \tag{3.19}$$

$$2^{-2K}\cdot a - 2b = \lambda_i \cdot b, \tag{3.20}$$

and thus,

$$\lambda_1 = 0, \quad \vec{P}^{(1)} = \vec{P}^{(e)} \tag{3.21}$$

$$\lambda_2 = -2(1+e^{-2K}), \quad \vec{P}^{(2)} = \begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \end{bmatrix} \tag{3.22}$$

$$\lambda_3 = -2e^{(-2K)}, \quad \vec{P}^{(3)} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ -1 \end{bmatrix} \tag{3.23}$$

$$\lambda_4 = -2, \quad \vec{P}^{4} = \begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \end{bmatrix} \tag{3.24}$$

$$\tag{3.25}$$

The time evolution of the average of a physical quantity $\langle Q(s_1, s_2)\rangle$ is obtained by averaging over the time- dependent distribution $P(s_1, s_2; t)$

$$Q(t) = \langle Q\rangle_t = \sum_{s_1=\pm1}\sum_{s_2=\pm1} Q(s_1+s_2)P(s_1, s_2; t). \tag{3.26}$$

Since we would like to calculate the time-evolution of the magnetization of the system, $Q = s_1 + s_2$ in our case, and we have

$$m(t) = \sum_{s_1=\pm1}\sum_{s_2=\pm1} (s_1+s_2)P(s_1, s_2; t) \tag{3.27}$$

Collecting the components, we have

$$\vec{P}(t) = \begin{bmatrix} \frac{e^K}{Z} + e^{-2(1+e^{-2K})t}\frac{e^K}{Z} + e^{-2e^{-2K}t}\frac{1}{2} \\ \frac{e^-K}{Z} - e^{-2(1+e^{-2K})t}\frac{e^K}{Z} \\ \frac{e^-K}{Z} - e^{-2(1+e^{-2K})t}\frac{e^K}{Z} \\ \frac{e^K}{Z} + e^{-2(1+e^{-2K})t}\frac{e^K}{Z} - e^{-2e^{-2K}t}\frac{1}{2} \end{bmatrix} \tag{3.28}$$

We have now all $P(s_1, s_2, t)$ and can evaluate $m(t)$ as given by 3.27. equation. We can notice that $s_1 + s + 2 = 0$ for the $\downarrow\uparrow$ and $\uparrow\downarrow$ states, while $s_1 + s_2 = 2$ for the $\uparrow\uparrow$ and $s_1 + s_2 = -2$ for the $\downarrow\downarrow$ states. Thus the sum reduces to the following expression

$$m(t) = 2[P(\uparrow\uparrow, t) - P(\downarrow\downarrow, t)]. \tag{3.29}$$

Using now the $\vec{P}(t)$ components from 3.28 matrix, we find

$$m(t) = 2e^{-2e^{-2K}t} \tag{3.30}$$

Thus the magnetization of the system relaxes exponentially with a relaxation time given as the inverse of one of the eigenvalues of the dynamical matrix

$$\tau_{relax} = \frac{1}{2}e^{2K} = \frac{1}{2}e^{\frac{2J}{k_BT}} \tag{3.31}$$

4 Emphasize my contribution

4.a N = 2 system

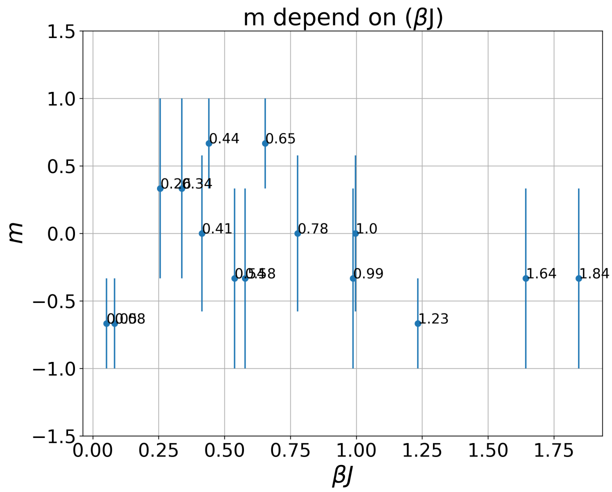

Figure 4.a.1:
Final state magnetization m depend on βJ, start with random value spins.

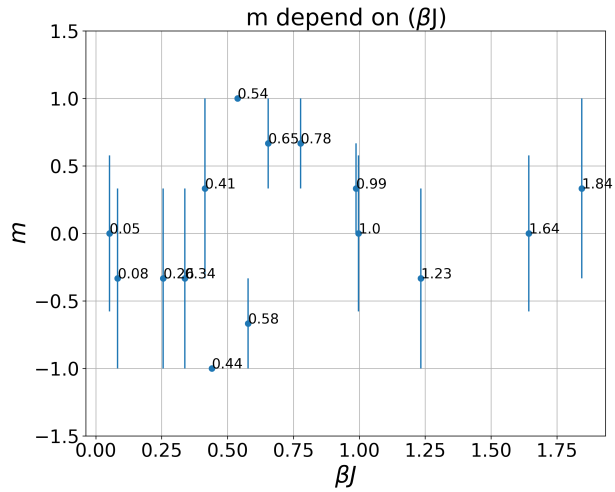

Figure 4.a.2:
Final state magnetization m depend on βJ, start with arranged value spins.

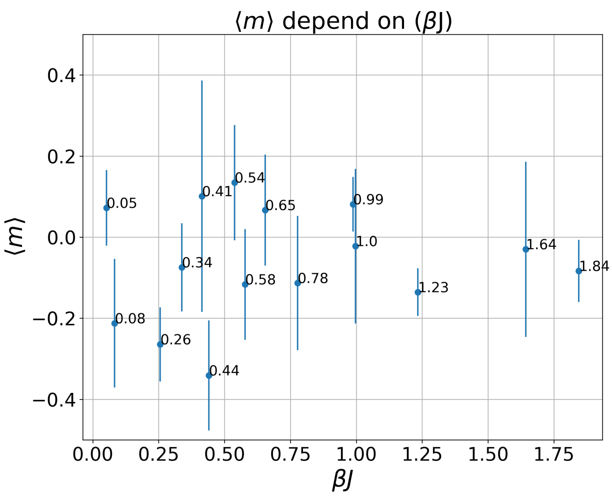

Figure 4.a.3:
Mean of magnetization $\langle m \rangle$ depend on βJ, start with random value spins.

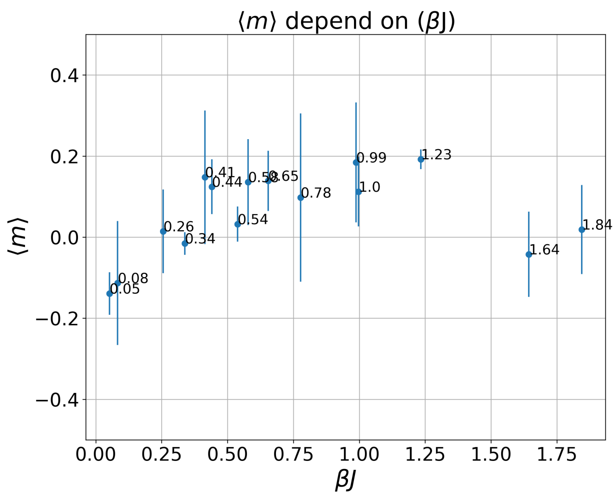

Figure 4.a.4:
Mean of magnetization $\langle m \rangle$ depend on βJ, start with arranged value spins.

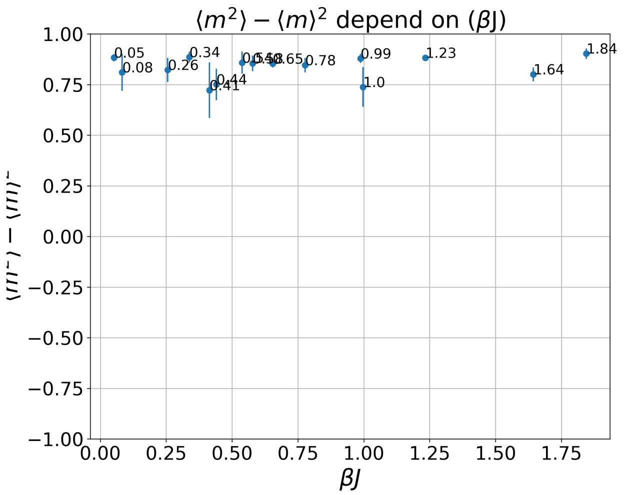

Figure 4.a.5:
The standard deviation of the mean of the magnetization $\langle m^2 \rangle - \langle m \rangle^2$ depend on βJ, start with random value spins.

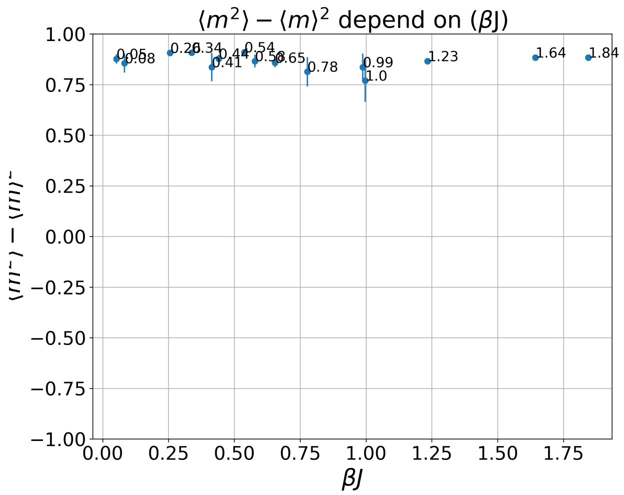

Figure 4.a.6:
The standard deviation of the mean of the magnetization $\langle m^2 \rangle - \langle m \rangle^2$ depend on βJ, start with arranged value spins.

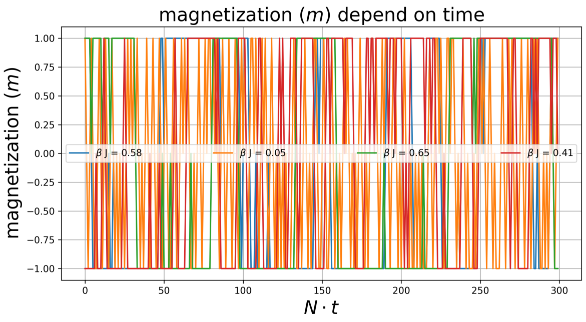

Figure 4.a.7:
The magnetization depend on t, start with random value spins.

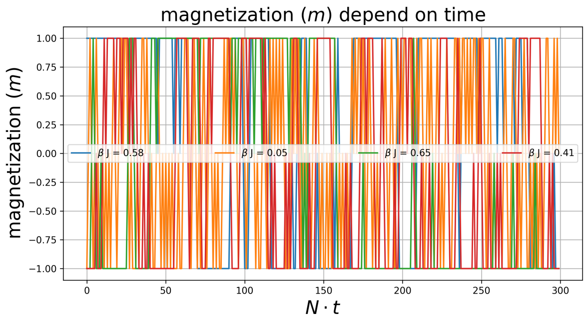

Figure 4.a.8:
The magnetization depend on t, start with arranged value spins.

4.b N = 10 system

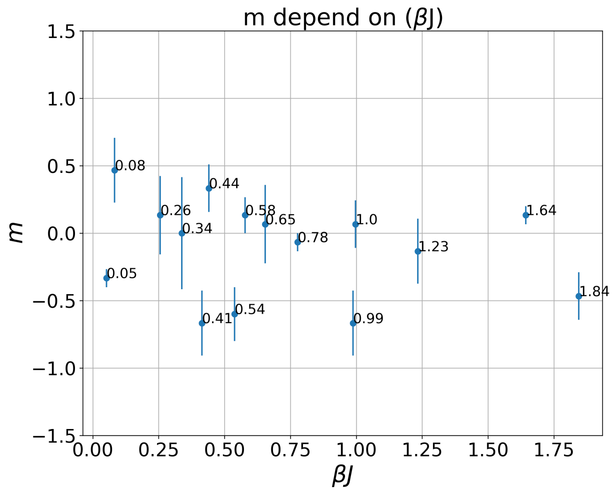

Figure 4.b.1:
Final state magnetization m depend on βJ, start with random value spins.

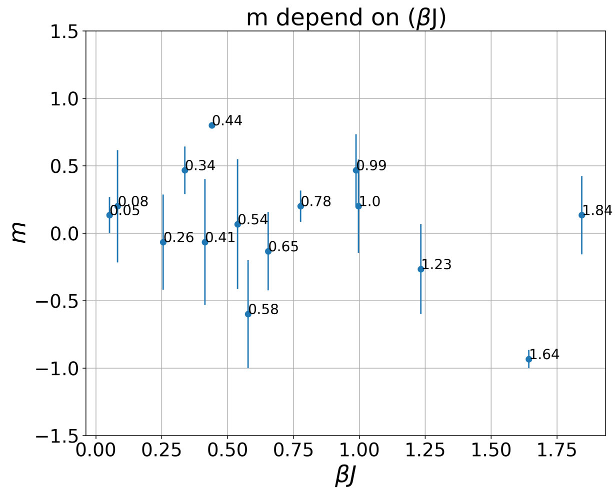

Figure 4.b.2:
Final state magnetization m depend on βJ, start with arranged value spins.

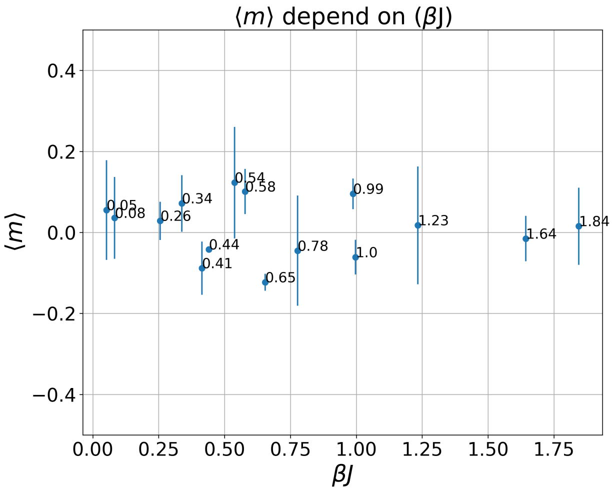

Figure 4.b.3:
Mean of magnetization $\langle m \rangle$ depend on βJ, start with random value spins.

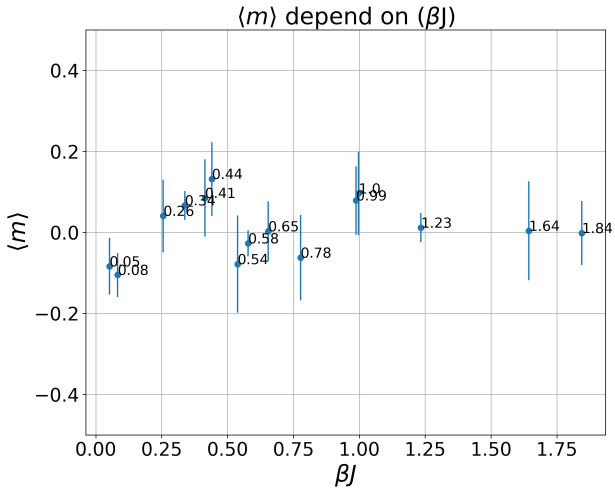

Figure 4.b.4:
Mean of magnetization $\langle m \rangle$ depend on βJ, start with arranged value spins.

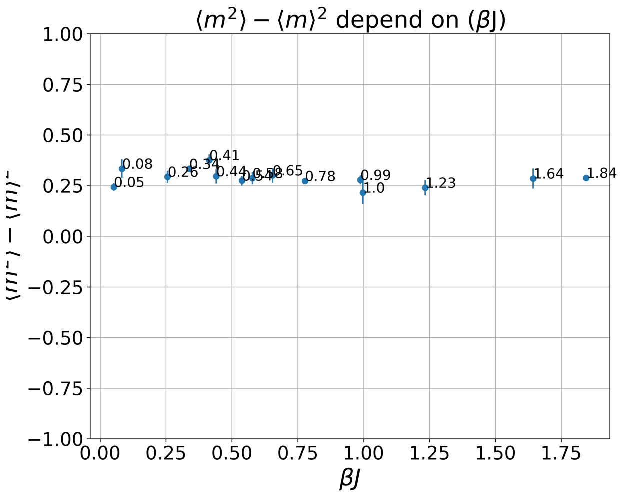

Figure 4.b.5:
The standard deviation of the mean of the magnetization $\langle m^2 \rangle - \langle m \rangle^2$ depend on βJ, start with random value spins.

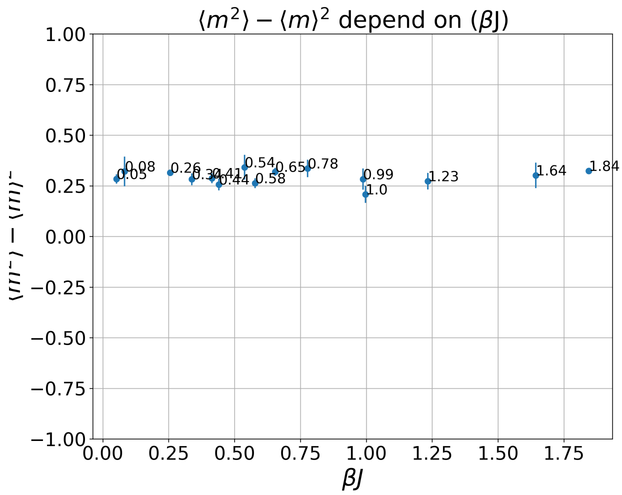

Figure 4.b.6:
The standard deviation of the mean of the magnetization $\langle m^2 \rangle - \langle m \rangle^2$ depend on βJ, start with arranged value spins.

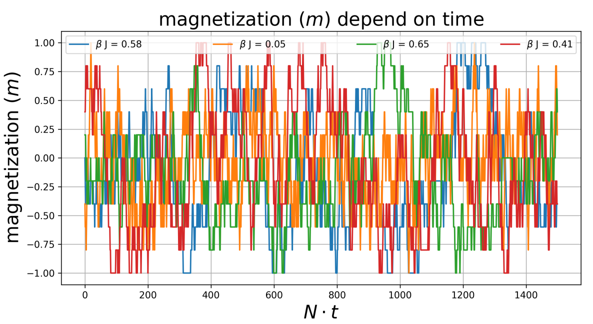

Figure 4.b.7:
The magnetization depend on t, start with random value spins.

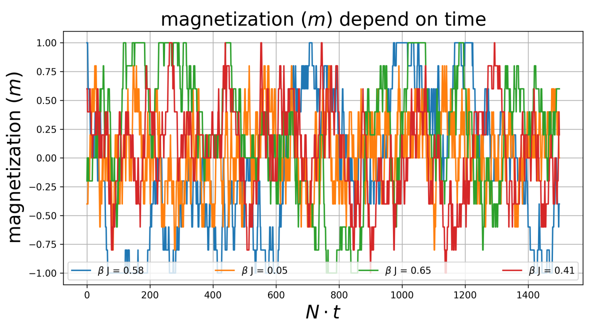

Figure 4.b.8:
The magnetization depend on t, start with arranged value spins.

4.c N = 20 system

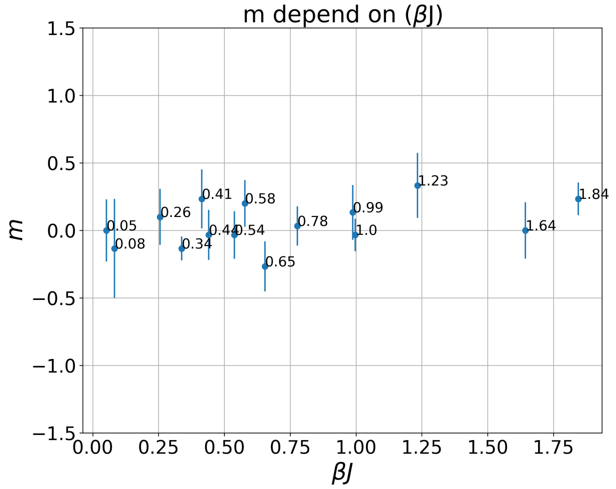

Figure 4.c.1:
Final state magnetization m depend on βJ, start with random spins.

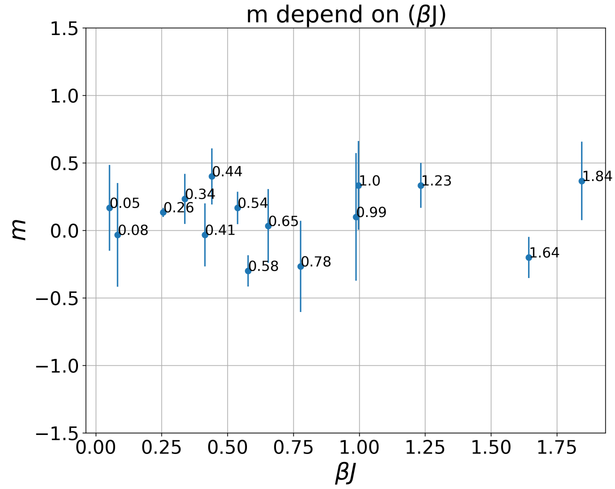

Figure 4.c.2:
Final state magnetization m depend on βJ, start with arranged value spins.

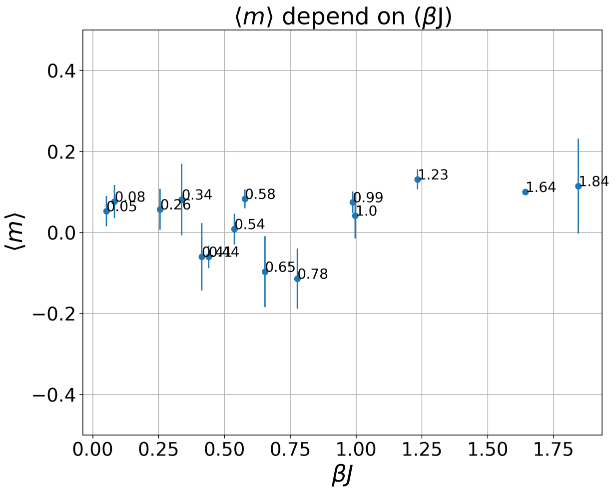

Figure 4.c.3:
Mean of magnetization $\langle m \rangle$ depend on βJ, start with random value spins.

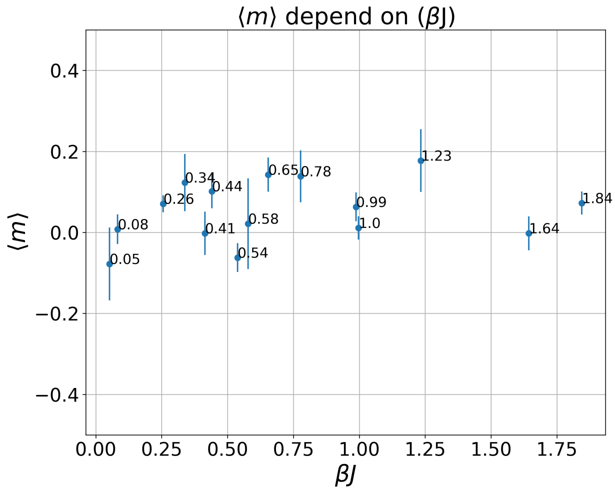

Figure 4.c.4:
Mean of magnetization $\langle m \rangle$ depend on βJ, start with arranged value spins.

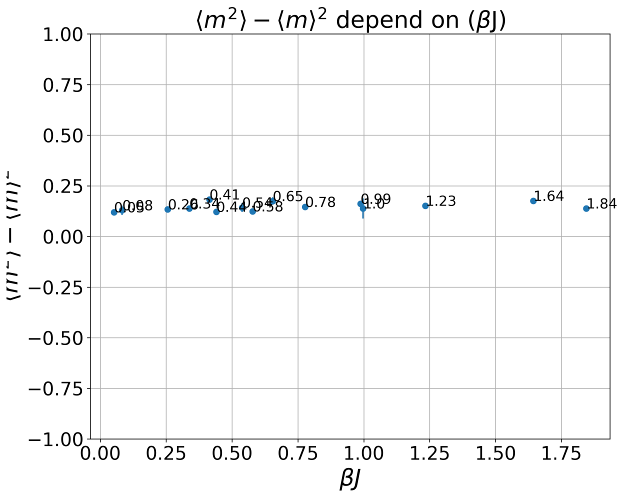

Figure 4.c.5:
The standard deviation of the mean of the magnetization $\langle m^2 \rangle - \langle m \rangle^2$ depend on βJ, start with random value spins.

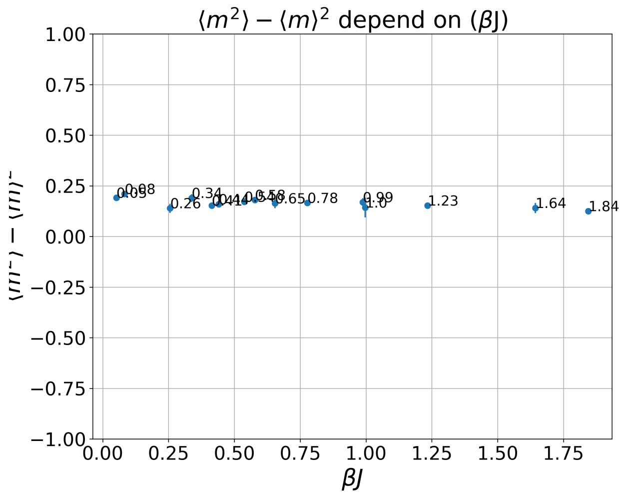

Figure 4.c.6:
The standard deviation of the mean of the magnetization $\langle m^2 \rangle - \langle m \rangle^2$ depend on βJ, start with arranged value spins.

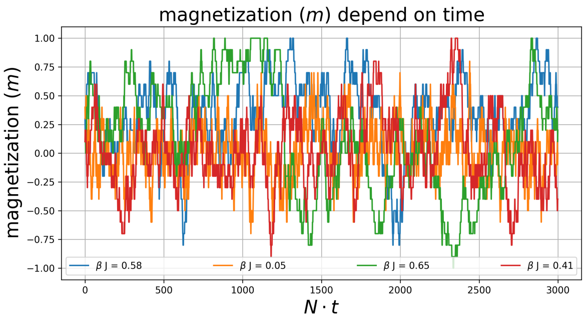

Figure 4.c.7:
The magnetization depend on t, start with random value spins.

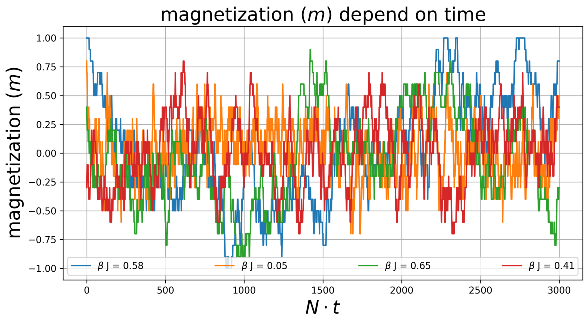

Figure 4.c.8:
The magnetization depend on t, start with arranged value spins.

4.d N = 50 system

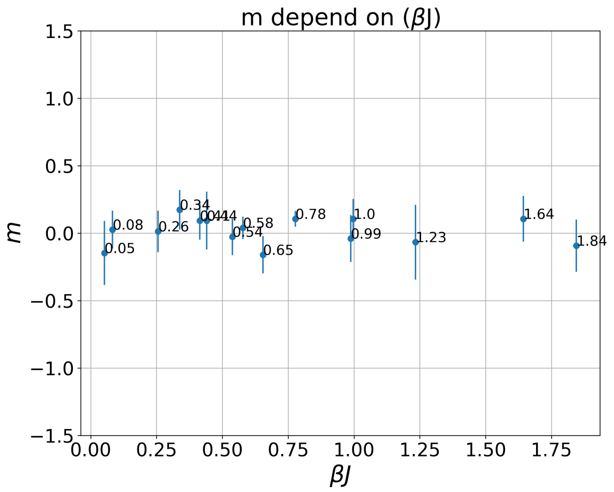

Figure 4.d.1:
Final state magnetization m depend on βJ, start with random value spins.

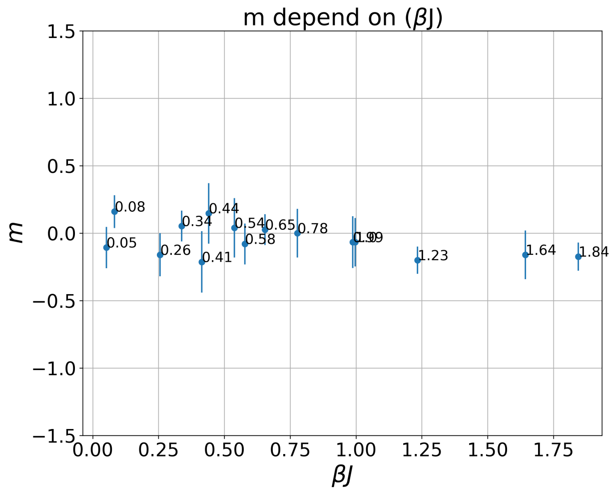

Figure 4.d.2:
Final state magnetization m depend on βJ, start with arranged value spins.

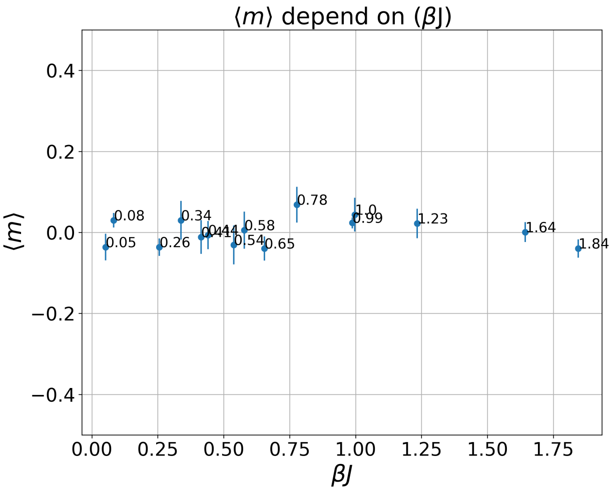

Figure 4.d.3:
Mean of magnetization $\langle m \rangle$ depend on βJ, start with random value spins.

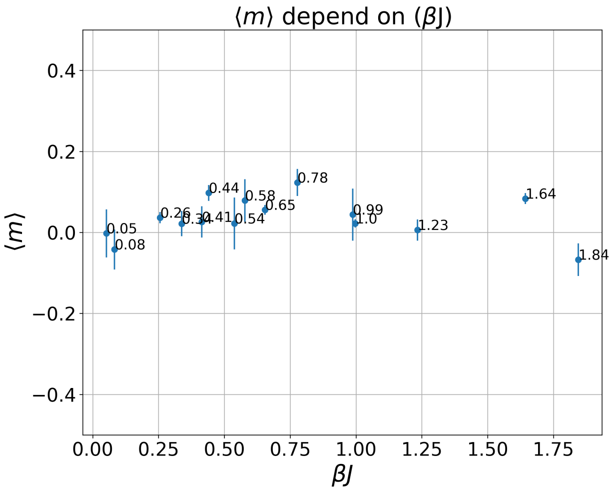

Figure 4.d.4:
Mean of magnetization $\langle m \rangle$ depend on βJ, start with arranged value spins.

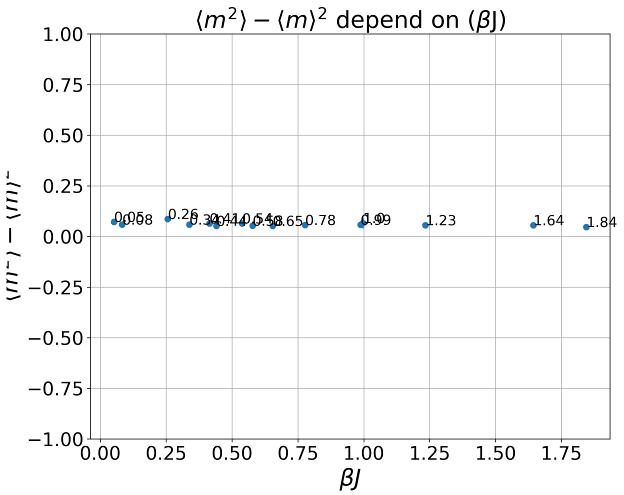

Figure 4.d.5:
The standard deviation of the mean of the magnetization $\langle m^2\rangle - \langle m\rangle^2$ depend on βJ, start with random value spins.

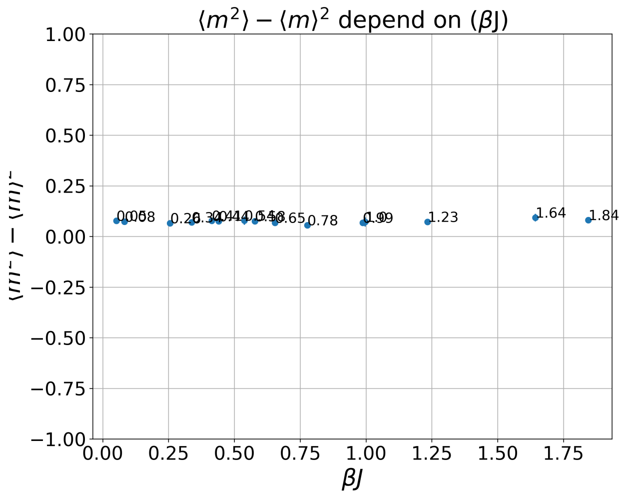

Figure 4.d.6:
The standard deviation of the mean of the magnetization $\langle m^2\rangle - \langle m\rangle^2$ depend on βJ, start with arranged value spins.

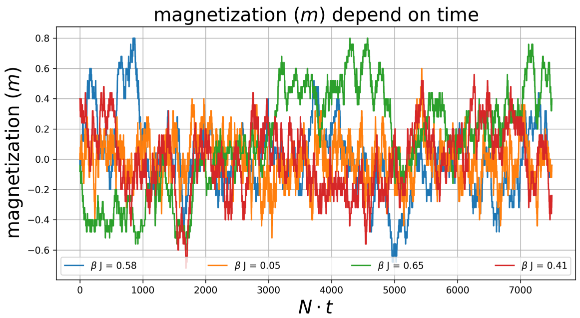

Figure 4.d.7:
The magnetization depend on t, start with random value spins.

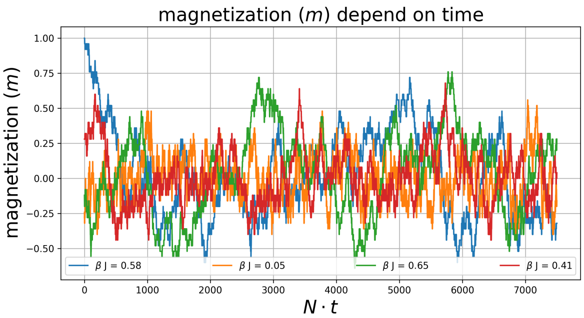

Figure 4.d.8:
The magnetization depend on t, start with arranged value spins.

4.e N = 350 system

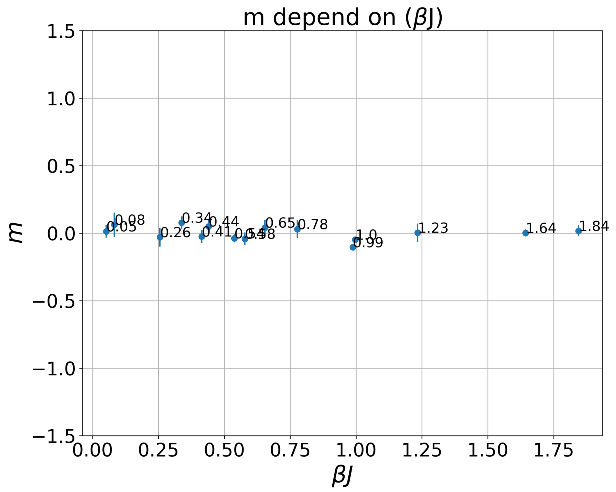

Figure 4.e.1:
Final state magnetization m depend on βJ, start with random value spins.

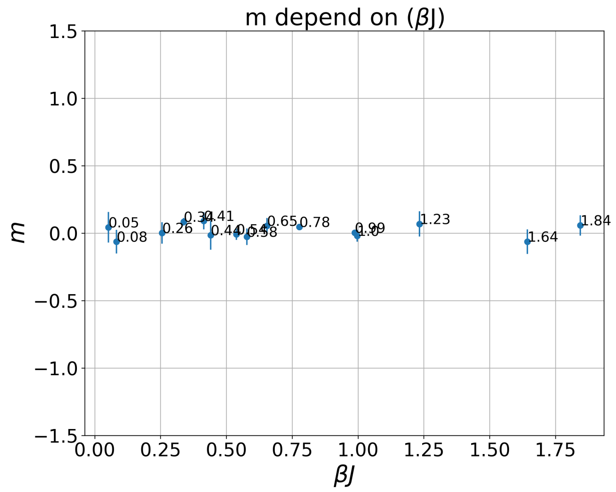

Figure 4.e.2:
Final state magnetization m depend on βJ, start with arranged value spins.

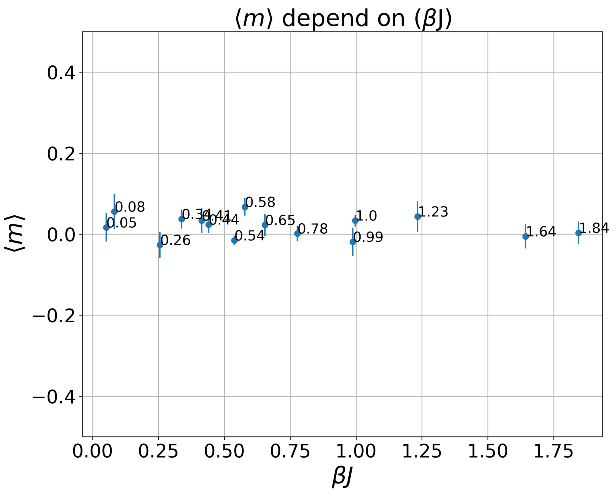

Figure 4.e.3:
Mean of magnetization $\langle m \rangle$ depend on βJ, start with random value spins.

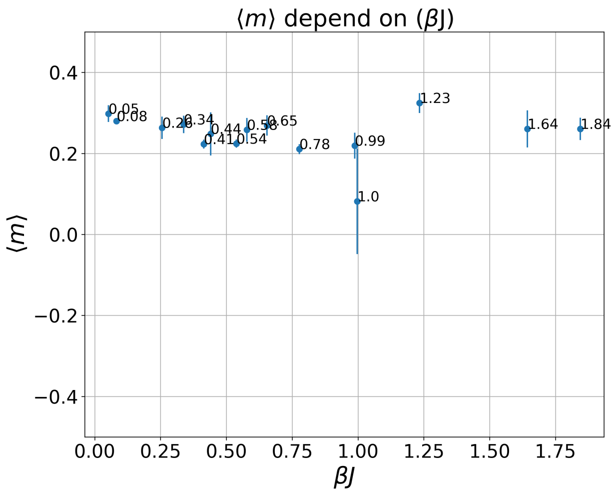

Figure 4.e.4:
Mean of magnetization $\langle m \rangle$ depend on βJ, start with arranged value spins.

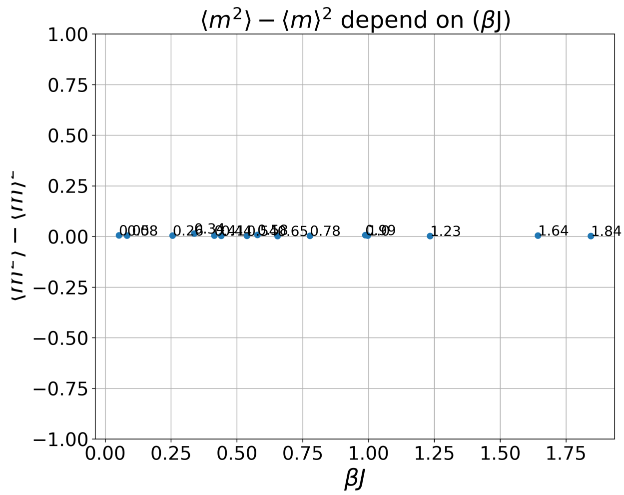

Figure 4.e.5:
The standard deviation of the mean of the magnetization $\langle m^2 \rangle - \langle m \rangle^2$ depend on βJ, start with random value spins.

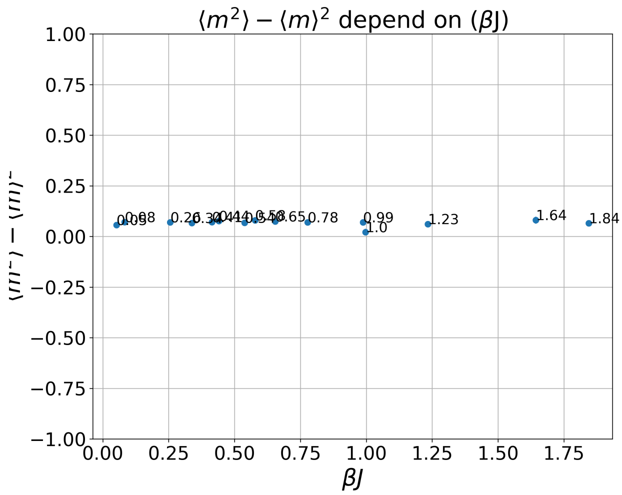

Figure 4.e.6:
The standard deviation of the mean of the magnetization $\langle m^2 \rangle - \langle m \rangle^2$ depend on βJ, start with arranged value spins.

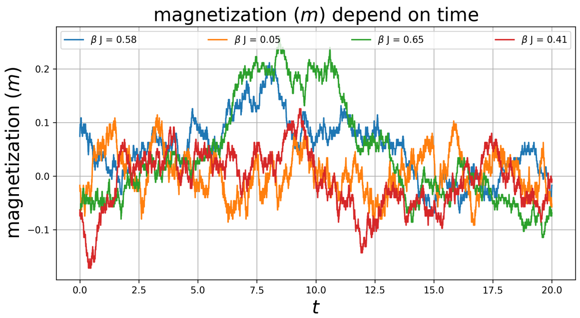

Figure 4.e.7:
The magnetization depend on t, start with random value spins.

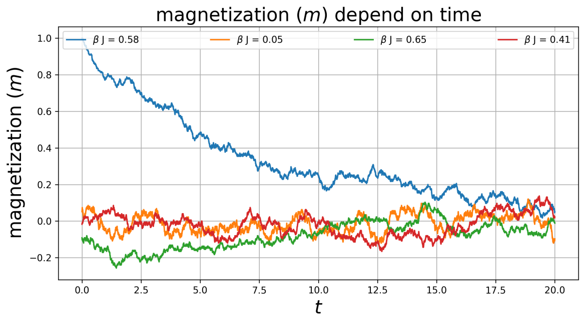

Figure 4.e.8:
The magnetization depend on t, start with arranged value spins.

5 Discussion

I ran the simulation with every βJ value four times ($t = 150$) to could calculate the average of results. I ran the simulation with random spins and with arranged spins as well to see what the difference between the two type of simulation. I examined and depicted the actual magnetization (m), mean of the magnetization $\langle m \rangle$ and the standard deviation of the mean of the magnetization $\langle m^2 \rangle - \langle m \rangle^2$.
I depicted the magnetization depend on time and we can see on every image that the magnetization (m) is fluctuates around the $m = 0$. We can see a linear relationship between m value and βJ, the higher βJ belongs to the higher protrusion. We can see from the simulation that belongs to bigger βJ the standard deviation.
During the increase the N, the final state magnetization is more closer to zero, end the error is also smaller, I do not see significant difference between the two type of starts. We can see the same result of the $\langle m \rangle$.
We can see significant difference between the average of the $\langle m^2 \rangle - \langle m \rangle^2$ if we examine it with different N. If we increase the N the value of the $\langle m^2 \rangle - \langle m \rangle^2$ is more closer to zero.
As we expected we could approach the theoretical relaxation if we increase the N. If we ran the command to $N = 350$ and $t = 20$, the magnetization depend on βJ is almost zero for every βJ as the theoretical figure show.
So if we have a macroscopic material where the $N = C \cdot 6,022 \cdot 10^{23}$ we can use the theoretical results. If we run the simulation with the random spins we got more closer results to the theoretical.

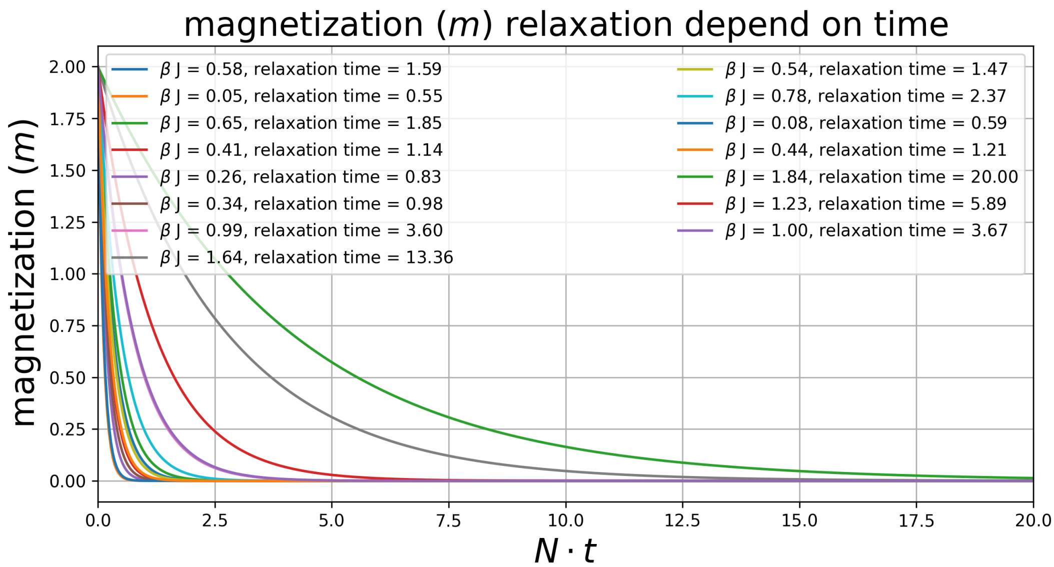

Figure 5..1:
The theoretical relaxation of magnetization(calculated by: 3.30.eq, 3.31.eq)