The correlation time

Now that you have experimented a bit with the setup and know how long you need to wait to have equilibrated samples, we need to find out how long you have to run the simulation *after equilibration* in order to determine physical quantities with reasonable statistics. For this we need to determine the *correlation time*, the time it takes before the system has forgotten its previous state. A particular example, is that we want it to have forgotten everything about the initial state.

The measurement of a physical quantity should then be determined by a simulation that is several correlation times long. To determine it, you can follow the behavior of the magnetization after the sample is equilibrated. The autocorrelation function $\chi(t)$ of the magnetization measures how much the magnetization at time t' is related to the magnetization at a time $t'+t$. If, for instance, the magnetization per spin at time t' is larger than its average, i.e. $m(t') > \langle m \rangle$, then, if t is smaller than the correlation time, it is also typically larger than average at $t'+t$, i.e. $m(t'+t) > \langle m \rangle$. On the other hand, if t is larger than the correlation time, then $m(t'+t)$ is equally likely positive or negative, independent of the value of $m(t')$. The so-called time-displaced autocorrelation function of the magnetization is given by

$$\begin{aligned} \chi(t) &= \int \left(m(t') - \langle m \rangle\right)\left(m(t'+t) - \langle m \rangle\right) dt' \qquad (1) \\ &= \int \left(m(t')\, m(t'+t) - \langle m \rangle^2\right) dt'. \end{aligned}$$

In principle to determine χ for all times t one needs to integrate over an infinite time but this is obviously not possible for a simulation. In addition, time in our setup is *discrete* and counts the Monte Carlo steps per lattice site (the sweeps). Let us call that total number of sweeps (after equilibration) $t_{\max}$. For this case the formula for the autocorrelation function is given by

$$\begin{aligned} \chi(t) &= \frac{1}{t_{\max}-t} \sum_{t'=0}^{t_{\max}-t} m(t')\, m(t'+t) \\ &\quad - \frac{1}{t_{\max}-t} \sum_{t'=0}^{t_{\max}-t} m(t') \times \frac{1}{t_{\max}-t} \sum_{t'=0}^{t_{\max}-t} m(t'+t)\,. \end{aligned}$$

The second term calculates $\langle m \rangle^2$; the choice of the two summations makes sure that the same subsets of the data are used as in the first term. This is

not strictly necessary but improves the behavior of $\chi(t)$.

You should find that the measured auto-correlation function falls off roughly exponentially

$$\chi(t) \approx \chi(0)\, e^{-t/\tau}.$$

where τ denotes the correlation time. Note, however, that there is an increase in statistical fluctuations in $\chi(t)$ for larger values of t. This reflects the fact that there are less and less intervals $[t', t'+t]$ to average over (small number statistics!). For long enough simulation the exponential function has decayed already to a very small value before these fluctuations become important. This allows to determine τ by integrating over the autocorrelation function:

$$\int_0^\infty \frac{\chi(t)}{\chi(0)} = \int_0^\infty e^{-t/\tau} dt = \tau.$$

How do we compute this integral in paractice? We replace the integration by a summation and simply stop the summation once $\chi(t) < 0$, as this signals the onset of poor statistics for longer times.

Thermal averages

Now if one wants to measure the thermal average of some quantity, e.g. the average magnetization, one needs to draw it many times. Computing the thermal average is relatively straightforward. But, computing the standard deviation of the mean is more tricky. The problem is that two samples drawn a distance of Δt sweeps apart, are *not independent* from each other if Δt is smaller than the correlation time τ. One can show that a natural choice to achieve statistical independence turns out to be $\Delta t = 2\tau$. Consequently the standard deviation of the mean is given by

$$\sigma = \sqrt{\frac{2\tau}{t_{\max}} \left(\langle m^2 \rangle - \langle m \rangle^2 \right)}$$

(Note that this corresponds to Eq. 5 of last lecture with N replaced by $t_{\max}/(2\tau)$!).
So even if you average over all sweeps, $t_{\max}$ in total with $t_{\max} \gg \tau$, the equation for σ accounts for the fact that you took only about $t_{\max}/\tau$ independent measurements.

We can now move to the main goal of this project. Having determined the equilibration and correlation time, we can calculate now properly the

equilibrium properties of the $N \times N = 50 \times 50$ system of spins.

We can begin with the magnetization which is most straightforward to implement. The only problem with the magnetization is that the system (well) below the critical temperature shows either a state with an overall positive or an overall negative magnetization, depending in which state the system settles in first. One way to avoid this problem is to calculate instead the average of the absolute value of the magnetization (per spin)

$$\langle |\ m\ | \rangle = \frac{1}{N^2} \langle |\ \sum_i s_i\ | \rangle.$$

We want to calculate the mean of this quantity and the standard deviation of the mean (see the equation for σ above) for a given temperature.

We also want to do the same for the energy per spin $e = E/N^2$.

Moving towards more complicated quantities, we want to determine the magnetic susceptibility per spin[1]:

$$\chi_M = \frac{\beta}{N^2} \frac{\partial \langle M \rangle}{\partial H} = \frac{\beta}{N^2} \left(\langle M^2 \rangle - \langle M \rangle^2 \right)$$

and the specific heat per spin

$$C = \frac{\partial E}{\partial T} = \frac{1}{N^2 k_B T^2} \frac{\partial^2 \ln Z}{\partial \beta^2} = \frac{1}{N^2 k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right).$$

and also estimate the error for these two quantities.

This is, however, a bit more challenging than for the cases of magnetization and energy. The reason is that—unlike for the former two quantities— you do not determine χ_M and C by averaging some measurements repeated many times over the course of the simulation. Instead these quantities are determined in a more complex way from those measurements.

In order to give a rough estimate of the error you can use the blocking method. You divide the measurement into successive blocks, each containing n measurements. For each block you determine χ and C. Assuming that blocks are independent from each other, the standard error is estimated in the usual way. How large should the blocks be? Obviously they need to be large enough such that a calculation of χ and C within a block averages over (much)

[1]Note the same χ as eq. 1!

more than a correlation time τ. Otherwise the fluctuations in magnetization and energy are severely underestimated, as e.g. $\langle M^2 \rangle$ and $\langle M \rangle^2$ are too similar in value. In addition, different blocks, even if they are neighbors, should be approximately independent, calling again for a block length (much) larger than τ. For the current system a reasonable value for the block length is 16τ, calling for a relatively long simulation time around the critical point (as a sufficient number of blocks is needed for proper averaging).

There are many possible ways to explore this system further[2]. Possibilities include:

- Study the effect of an external magnetic field.
- Study the entropy of the system (Recall $\frac{C}{T} = \frac{\partial S}{\partial T}$).
- Implement so-called "cluster flipping algorithms" (e.g. the Wolff algorithm[3]) that are more suitable to explore the region around the critical point where large clusters of parallel spins occur. These algorithms do not suffer from the dramatic critical slowing down around the critical point which we observed for the simple spin-flipping algorithm we used.
- Explore more systematic methods to estimate errors for quantities like χ_M and C, especially the *bootstrap* and the *jackknife* methods.
- Extract the values for the critical exponents ν which occur in the power laws of the various physical quantities ($\langle A \rangle \approx (T_c - T)^\nu$) around the critical point for the correlation length, magnetic susceptibility, specific heat, spontaneous magnetization). This can be achieved in a systematic way through the so-called *finite size scaling method*.

[2]See for instance the excellent book "Monte Carlo Methods in Statistical Physics" by M. E. J. Newman and G. T. Barkema

[3]Wolff U., "Collective Monte Carlo Updating for Spin Systems", Phys. Rev. Lett., 1989, **62**, 361

Final milestones:

Calculate the correlation time τ as a function of temperature for the same temperature points as in the last lecture ($T = 1.0$ to $T = 4.0$ in steps of 0.2, in units where $J = k_B = 1$). Important is that you only calculate this quantity *after* the system is equilibrated.

Plot τ as a function of temperature. You should observe that τ peaks around the critical temperature ($T_c = 2.269$), an effect called critical slowing down.

Compute the mean and standard deviation as a function of temperature of the following quantities:

- Magnetization per spin m,
- Energy per spin e,
- Magnetic susceptibility per spin χ_M,
- Specific heat per spin C.

Comment on your findings.

Extensions

There are many ways the project can be extended. This can either be by including more physics, running a larger system, or by extending the analysis.

One possibility is to extend the problem by considering the 3D Ising model. In 3D the model has no known analytic solution. The critical temperature can nevertheless be found using Monte-Carlo simulations. Can you find it?

A second option is to include the external magnetic field that we ignored in the Hamiltonian. How does the system react? Does the critical temperature change?

Finally, one of the properties of the model was that we only consider directly neighbouring spins in the grid. What happens if the Hamiltonian is extended to include further neighbours? e.g. neighbours at a distance of two spins. What happens if the coupling term (J) depends on distance, e.g. is half as large for neighbours in the second layer?