

1 Discussion

1.1 Ising model: simulation over temperature

As presented in Results (see table ?? and ??), when using periodic boundary conditions and $T = 1.0(kT/J)$, 10^6 Monte Carlo cycles gives high precision results. The energy and magnetisation have a precision of three leading digits after the decimal point, while it is a little less for susceptibility and heat capacity.

When using a random starting configuration the precision increases slightly compared with the specific one for some of the parameters, especially for the susceptibility.

For further computations we have used $10^4 - 10^7$ Monte Carlo cycles in order to not have too time consuming computation.

1.2 20×20 lattice

From Figure ?? and ?? one sees the impact of the different parameters, initialisation and temperature, before reaching equilibrium for different Monte Carlo cycles.

For $T = 1.0(Jk/T)$ the predetermined starting configuration, the energy and magnetisation stabilizes is already really stable after only a few Monte Carlo cycles (take a close look at the y-axis). It is easy to see that at the first Monte Carlo cycle the magnetisation is one (because all the spins are pointing the same way). Then one spin flips and the energy changes slightly. After a while it is almost no longer energetically favourable to flip spins. While for the random initialisation it takes more time/Monte Carlo cycles before stabilizing (take a look at the y-axis, it is 3 orders of magnitude larger than the predetermined). For easier comparison it would be convenient to have the axes more alike.

To summarize the ordered starting point seems to stabilize the fastest for both temperatures (energy a bit faster than magnetisation). This is expected, because at low temperatures, which we are dealing with, one would expect a high order at equilibrium (from eg. Gibbs free energy). So when we start with a high order, we are already close to equilibrium.

There is also a difference between the different temperatures, which is also expected from thermodynamics. A system of higher temperature is expected to reach equilibrium at a less ordered state. This is quite evident in both the ordered and the random initialisation.

When studying the accepted spin configurations per Monte Carlo cycle (see Figure ??) the same trend as above occurs. At low temperature and ordered starting point we are already close to equilibrium and therefore the number of accepted spins increases steadily with the number of Monte Carlo cycles.

1.3 Analyzing the probability distribution

While the probability distribution for the higher temperature was really good, it seemed rather odd for the low temperature. One would think that since most energies are at their lowest, the histogram would take the shape of an inverse exponential curve. And while this is the case we still have large gaps between the energies. For example from -800 to -794 it looks like there isn't a single lattice observed.

This must be because the energy change when flipping a spin can be 4J, or 8J. This correlates to the histogram beautifully. Another thing to mention is that at lower temperatures, the spins are having a harder time to flip without causing higher energy, thus the flip will happen more seldom and trap the lattice in the already set energy state.

The standard deviation for the low temperature histogram does not give us anything. It is only relevant for a gaussian curve, like the one for the higher temperature. Thus it is irrelevant to compare the standard deviation to the calculated variance.

On the flipside, the variance of the higher temperature has a good correspondence to the calculated variance, with a deviation of about 6.2%.

1.4 Numerical studies of phase transitions

From the plots ?? and ?? it is clear that something is happening around $T = 2.3$. You can also see that a bigger lattice reacts more to the temperature than the smaller lattice.

1.5 Extracting the critical temperature

The most difficult part was to set the critical temperatures for the different lattice sizes. As explained, we used the FWHM technique, but this is also prone to error. However with this technique we got within 0.3% of Lars Onsager's exact result, which is quite good.