

Prosjekt 4

Benedicte Allum Pedersen, Emil Heland Broll
Fredrik Oftedal Forr

Abstract

Si meg, hva betyr adjø?
Er det bare trist?
Noe som sårer deg?
Tro meg, vi skal ta adjø
Ikke sånn som sist
Da jeg gikk fra deg

Introduction

In this project we will study the Ising model in two dimensions. This is a model which is used to simulate phase transitions. The model exhibits a phase transition from a magnetic phase to a phase with zero magnetization. We study electrons in a lattice which is a binary system because each electron only can take two values, spin up or spin down.

The energy we get from the Ising model without an externally applied magnetic field is given by:

$$E = -J \sum_{\langle kl \rangle}^N S_k S_l$$

where $s_k, s_l = \pm 1$ and represents classical spin values. N is the total number of spins and J is a coupling constant expressing the strenght of the interactions between neighboring spins. $\langle kl \rangle$ indicates that we sum over the spins of the nearest neighbors. We apply periodic boundary conditions as well as the Metropolis algorithm. We also assume that we have a ferromagnetic ordering, so $J > 0$.

Method

When calculating the degenerate energies for the case of 2x2, we start with the equation $E_i = -J \sum_{\langle kl \rangle}^2 s_k s_l$

The case for all spin up looks like this $\begin{array}{cc} \uparrow & \uparrow \\ \uparrow & \uparrow \end{array}$

And the equation will be.

$$\begin{aligned}
E_1 &= -J \sum_{\langle kl \rangle}^2 s_k s_l \\
&= -J((s_1 s_2 + s_1 s_3) + (s_2 s_1 + s_2 s_4) + (s_3 s_1 + s_3 s_4) + (s_4 s_3 + s_4 s_2)) \\
&= -J((1 + 1) + (1 + 1) + (1 + 1) + (1 + 1)) \\
E_1 &= -8J
\end{aligned}$$

The reason why the same interaction is included several times is because of the unit cell repeating itself to infinity in both x and y direction. Therefore the s_1 will interact with s_2 and s_3 inside the unit cell, and s_2 and s_3 "outside" the unit cell.

When this is known for all the degenerate energies we can calculate the value of the partition function.

$$z = \sum_{i=1}^{2^n} e^{-\beta E_i}$$

In our case we have $n = 4$ since we have a 2x2 lattice.

$$\begin{aligned}
z &= \sum_{i=1}^{2^4} e^{-\beta E_i} \\
z &= e^{-\beta E_1} + e^{-\beta E_2} + \dots + e^{-\beta E_{16}} \\
z &= e^{8\beta J} + 4e^{-\beta \cdot 0} + 2e^{-8\beta J} + 4e^{-\beta \cdot 0} + 4e^{-\beta \cdot 0} + 4e^{-\beta \cdot 0} + e^{8\beta J} \\
z &= 2e^{8\beta J} + 2e^{-8\beta J} + 16
\end{aligned}$$

This gives us the ability to calculate the expectation value of the energy $\langle E \rangle$

$$\langle E \rangle = \sum_i \frac{E_i e^{-\beta E_i}}{z}$$

We know we have several energy values which is zero. If we do not write these we get

$$\begin{aligned}
&= \frac{-8J e^{8\beta J} + 2(8J e^{-8\beta J}) + (-8J) e^{8\beta J}}{2e^{8\beta J} + 2e^{-8\beta J} + 16} \\
&= \frac{16J(e^{-8\beta J} - e^{8\beta J})}{2(e^{8\beta J} + e^{-8\beta J} + 8)} \\
&= 8J \frac{e^{-8\beta J} - e^{8\beta J}}{e^{8\beta J} + e^{-8\beta J} + 8}
\end{aligned}$$

Thus

$$\begin{aligned}
\langle E \rangle^2 &= \left(8J \frac{e^{-8\beta J} - e^{8\beta J}}{e^{8\beta J} + e^{-8\beta J} + 8} \right)^2 \\
&= 64J^2 \frac{(e^{-8\beta J} - e^{8\beta J})^2}{(e^{8\beta J} + e^{-8\beta J} + 8)^2} \\
&= 64J^2 \frac{e^{-16\beta J} + e^{16\beta J} + 2}{e^{-16\beta J} + e^{-16\beta J} + 16e^{-8\beta J} + 16e^{8\beta J} + 66}
\end{aligned}$$

At the same time we calculate $\langle E^2 \rangle$

$$\begin{aligned}
\langle E^2 \rangle &= \sum_i^{2^n} \frac{E_i^2 e^{-\beta E_i}}{z} \\
&= \frac{64J e^{8\beta J} + 2(64J e^{-8\beta J}) + 64J e^{8\beta J}}{2e^{8\beta J} + 2e^{-8\beta J} + 16} \\
&= \frac{128J e^{8\beta J} + 128J e^{-8\beta J}}{2e^{8\beta J} + 2e^{-8\beta J} + 16} \\
&= \frac{64J e^{8\beta J} + 64J e^{-8\beta J}}{e^{8\beta J} + e^{-8\beta J} + 8}
\end{aligned}$$

We use this to calculate the standard deviation

$$\begin{aligned}
\sigma_E^2 &= \langle E^2 \rangle - \langle E \rangle^2 \\
&= \frac{64J e^{8\beta J} + 64J e^{-8\beta J}}{e^{8\beta J} + e^{-8\beta J} + 8} - 64J^2 \frac{e^{-16\beta J} + e^{16\beta J} + 2}{e^{-16\beta J} + e^{-16\beta J} + 16e^{-8\beta J} + 16e^{8\beta J} + 66}
\end{aligned}$$

When this is known we can also calculate the heat capacitace.

$$\begin{aligned}
C_v &= \frac{\sigma_E^2}{k_b T} \\
&= \frac{\frac{64J e^{8\beta J} + 64J e^{-8\beta J}}{e^{8\beta J} + e^{-8\beta J} + 8} - 64J^2 \frac{e^{-16\beta J} + e^{16\beta J} + 2}{e^{-16\beta J} + e^{-16\beta J} + 16e^{-8\beta J} + 16e^{8\beta J} + 66}}{k_b T}
\end{aligned}$$