1. Domain walls in Ising model

\((5 + 5 + 5 + 10 + 5 + 10 + 20 = 60\) Punkte, schriftlich\)

(a) The energy of a state with a domain wall is just

\[- (N - 1)J + 2J. \quad (1)\]

There are \(N - 1\) positions where a domain wall can sit. The partition function with the account of states with a single domain wall reads

\[Z = Z_0 + \delta Z = e^{(N-1)\beta J} \left[1 + (N - 1)e^{-2\beta J}\right]. \quad (2)\]

(b) Due to fixing of spin \(\sigma_1\) to 1 the positions of domain walls immediately determine the spins. The energy of a state with \(m\) domain walls is

\[- NJ + 2Jm. \quad (3)\]

The number of states with \(m\) domain walls is just the number of ways to choose \(m\) places where we put a domain wall among available \(N - 1\) places.

\[Z = e^{(N-1)\beta J} \sum_{m=0}^{N-1} e^{-2J\beta \Gamma(m)} = e^{(N-1)\beta J} (1 + e^{-2\beta J})^{N-1} \quad (4)\]

In thermodynamic limit we reproduce the results of exercise sheet 8.

\[Z = \left[2 \cosh \beta J\right]^N \quad (5)\]

(d) Suppose we have a domain wall between spin \(k\) and \(k + 1\). It means that we have exactly \(N - k\) spins down in the system. The average number of spins down is

\[N_- = \frac{\exp((N - 1)\beta J - 2J\beta) \sum_{k=1}^{N-1} (N - k)}{\exp(NJ\beta) + (N - 1) \exp(N\beta J - 2\beta J)} = \frac{\exp(-2J\beta)N(N - 1)}{2[1 + (N - 1) \exp(-2\beta J)]} \quad (6)\]

Obviously, \(N_- \to 1/2N\) in thermodynamic limit.

(e) The spin \(\sigma_1\) is fixed in our system. On the other hand in state with \(m\) domain walls \(\sigma_N = (-1)^m\). Thus

\[\langle \sigma_1 \sigma_N \rangle = \frac{1}{Z} \sum_{m=0}^{N-1} (-1)^m \exp[(N-1)\beta J - 2Jm\beta] \Gamma[m] = \frac{1}{Z} \exp((N-1)\beta J) [1 - \exp(-2J\beta)]^{N-1} \quad (7)\]

In thermodynamic limit

\[\langle \sigma_1 \sigma_N \rangle = \left[\tanh \frac{J}{k_B T}\right]^N = e^{-N/\xi}, \quad \xi = - \frac{1}{\ln \tanh \frac{J}{k_B T}}. \quad (8)\]
(f) The excitation with smallest energy is just a single flipped spin. The energy of such a state (we concentrate on the thermodynamic limit and omit the boundary terms in the energy) is

$$-2NJ + 8J$$  \hspace{1cm} (9)

Average number of spins down reads

$$N_- = \frac{1}{Z} N \exp(2NJ\beta - 8J\beta)$$  \hspace{1cm} (10)

$$Z = \exp(2NJ\beta) [1 + N \exp(-8J\beta)]$$  \hspace{1cm} (11)

If $Ne^{-8J\beta} \ll 1$ we get

$$N_- \approx Ne^{-8J\beta}.$$  \hspace{1cm} (12)

In the opposite limit $N_- \approx 1$. Thus, in this approximations $N_-$ is always smaller then 1.

Obviously, $N_-$ is an extensive quantity and should be proportional to $N$. Thus, our answer is actually valid only in the limit $Ne^{-8J\beta} \ll 1$. We can improve it slightly by considering the configurations where arbitrary number of single-spin domains are present and neglecting interaction between them. This analogous to the ideal gas approximation. We then get

$$Z = e^{2NJ\beta} \sum_{m=0}^{\infty} \frac{1}{m!} N^m e^{-8mJ\beta} = \exp \left[ 2NJ\beta + Ne^{-8J\beta} \right]$$  \hspace{1cm} (13)

$$N_- = \frac{1}{Z} \sum_{m=0}^{\infty} \frac{1}{m!} N^m e^{-8mJ\beta} = \frac{Ne^{-8J\beta}}{Z} \exp \left[ 2NJ\beta + Ne^{-8J\beta} \right] = Ne^{-8J\beta}$$  \hspace{1cm} (14)

We see once again that $N_-/N \ll 1$ at low temperatures.

(g) So far we neglected completely the possibility of having domains of spin up with more than one spin (or equivalently the possibility of domain walls with length larger than 4). Let us show that the contribution of such configurations is negligible at low temperatures. The energy of a domain wall of length $m$ is just $2mJ$. How many different domain walls exist in the system? We can estimate it as follows. Lets start a domain wall somewhere and build it step by step. At each step we will have 3 options how to continue the domain wall (forward, right or left). We have also $N$ points to start the domain wall. Thus, we estimate the number of different domain walls as $3mN$. This is an estimate from above. It does not take into account the fact that a domain wall is always closed and after $m$ steps we should return to the point we started from. Thus, we have an estimate for the contribution of configurations with a single domain wall of length $m$ into the partition function

$$\delta Z_m < 3^m e^{-2mJ\beta} N$$  \hspace{1cm} (15)

We see that at low temperatures $Z_m$ decays monotonously as a function of $m$. Thus, the simplest single-spin domains are indeed most important.

2. Infinite-range interaction and mean-field theory.

(10 + 10 + 10 = 40 Punkte, mündlich)
(a) We have for the partition function
\begin{equation}
Z = \sum_\sigma \exp \left[ \beta \mathcal{H} \sum_i \sigma_i \right] \exp \left[ J \frac{\beta}{2N} \sum_{i,j} \sigma_i \sigma_j \right] = \sum_\sigma \exp \left[ \beta \mathcal{H} \sum_i \sigma_i \right] \exp \left[ J \frac{\beta}{2N} \left( \sum_i \sigma_i \right)^2 \right] = \sqrt{\frac{N \beta}{2\pi J}} \int dh \sum_\sigma \exp \left[ \beta \mathcal{H} \sum_i \sigma_i \right] \exp \left[ - \frac{\beta Nh^2}{2J} + \beta h \sum_i \sigma_i \right]. \quad (16)
\end{equation}

(b) After the Hubbard-Stratonovich transformation we can sum over the spins independently
\begin{equation}
Z = \sqrt{\frac{N \beta}{2\pi J}} \int dh \sum_\sigma \exp \left[ - \frac{\beta Nh^2}{2J} \right] \sum_\sigma \exp \left[ \beta (h + \mathcal{H}) \sum_i \sigma_i \right] = \sqrt{\frac{N \beta}{2\pi J}} \int dh \exp \left[ - \frac{\beta Nh^2}{2J} \right] [2 \cosh (h + \mathcal{H}) \beta]^N. \quad (17)
\end{equation}

The partition function can be written as
\begin{equation}
Z = \sqrt{\frac{N \beta}{2\pi J}} \int dh \exp[-\beta \mathcal{G}(\mathcal{H}, T, h)] \quad (18)
\end{equation}
\begin{equation}
\mathcal{G}(\mathcal{H}, T, h) = \frac{Nh^2}{2J} - k_B T N \ln [2 \cosh (h + \mathcal{H}) \beta] \quad (19)
\end{equation}

The function $\mathcal{G}$ is proportional to the number of particles. At large $N$ only small vicinity of minimum of $\mathcal{G}$ is important and the integration can be done by the saddle-point method. The saddle-point equation reads
\begin{equation}
\frac{h}{J} = \tanh \beta (h + \mathcal{H}) \quad (20)
\end{equation}

If we identify now $h = \mathcal{H}_{\text{eff}} - \mathcal{H}$ we get
\begin{equation}
\frac{\mathcal{H}_{\text{eff}} - \mathcal{H}}{J} = \tanh \beta \mathcal{H}_{\text{eff}}. \quad (21)
\end{equation}

The field $\mathcal{H}_{\text{eff}}$ is an effective field felt by a spin due to the combined effect of external magnetic filed and all the other spins.

(c) Let $h_0(T, \mathcal{H})$ be the solution of the saddle-point equation
\begin{equation}
\frac{h}{J} = \tanh \beta (h + \mathcal{H}). \quad (22)
\end{equation}

To compute the integral we write $h = h_0 + \delta h$ and expand the function $\mathcal{G}(h, T, \mathcal{H})$ to the second order in $\delta h$.
\begin{equation}
\mathcal{G} = \frac{h_0^2 N}{2J} + \frac{k_B T N}{2} \ln \frac{J^2 - h_0^2}{4J^2} + \frac{N(J + h_0^2 \beta - J^2 \beta)}{2J^2} \delta h^2. \quad (23)
\end{equation}

We see now explicitly that the fluctuations $\delta h$ are suppressed by $N \gg 1$. We evaluate the remaining gaussian integral over $\delta h$ and find the Gibbs free energy (only extensive part is interesting)
\begin{equation}
G(T, \mathcal{H}) = \mathcal{G}(h_0(T, \mathcal{H}), T, \mathcal{H}) = \frac{h_0^2 N}{2J} + \frac{k_B T N}{2} \ln \frac{J^2 - h_0^2}{4J^2}. \quad (24)
\end{equation}
Abbildung 1: Graphical solution of the saddle-point equation and function \( G \) in non-zero field \( \mathcal{H} \) at high temperatures \( J\beta < 1 \)

Here \( h_0 = h_0(T, H) \) is defined by the equation

\[
\frac{h_0}{J} = \tanh \beta (h_0 + \mathcal{H}).
\]  

(25)

Let us now discuss in more detail the saddle-point solution \( h_0 \). We start with the consideration of \( \mathcal{H} = 0 \). We have the equation.

\[
\frac{h}{J} = \tanh \beta h
\]

(26)

We can solve this equation graphically. Plotting \( \frac{h}{J} \) and \( \tanh \beta h \) on the same plot as functions of \( h \) we observe the following simple facts. At high temperatures, \( J/k_B T < 1 \). The only solution of the equation is \( h = 0 \). This corresponds to the fact that at high temperatures the spins are fluctuating strongly and their joined action on the given spin vanishes due to averaging.

At \( J/k_B T > 1 \) we get two solutions \( \pm h_0 \) and, of course a trivial solution \( h = 0 \). Correspondingly, the function \( G() \) has two (degenerate) minima at \( h = \pm h_0 \) and a maximum at \( h = 0 \). Computing the integral we should limit our the integration to the vicinity of one of the two minima of \( G \). This is the spontaneous symmetry breaking. To understand this point formally we can imaging that we have an infinitesimally small by finite external field \( \mathcal{H} \) in the system. This field will break the symmetry between the minima and make one of the minima slightly deeper then the other (which one depends on the sign of \( \mathcal{H} \)). Since \( G \) is proportional to the number of particles in the system and stays in the exponent. The contribution of the minimum with higher value of \( G \) will be strongly suppressed even for extremely small \( \mathcal{H} \).

Let us now include finite field \( \mathcal{H} \) into consideration. We assume for definiteness that \( \mathcal{H} \) is positive. At high temperatures, \( J/k_B T < 1 \), we get again only one minimum in \( G \).

At low temperatures and small magnetic field we get two minima, one of which is deeper and should be take into account.

At low temperatures and sufficiently large \( \mathcal{H} \) we are again in the situation with one minimum.

Let us now find the magnetization in the system. We have

\[
\frac{m}{N} = -\frac{1}{N} \partial_H G(H, T) = -\partial_{h_0} \left[ \frac{h_0^2}{2J} + \frac{k_B T}{2} \ln \frac{J^2 - h_0^2}{4J^2} \right] \partial_H h_0 = - \left[ \frac{h_0}{J} + \frac{h_0}{(h_0^2 - J^2) \beta} \right] \partial_H h_0
\]

(27)
Abbildung 2: Graphical solution of the saddle-point equation and function $G$ in non-zero but small field $H$ and low temperatures $J\beta > 1$.

Abbildung 3: Graphical solution of the saddle-point equation and function $G$ relatively large field $H$ and low temperatures $J\beta > 1$.

To find $\partial_H h_0$ we use the saddle point equation (differentiate it with respect to $H$) We find

$$\frac{\partial_H h_0}{J} - \frac{\beta(1 + \partial_H h_0)}{\cosh^2 \beta(h_0 + H)} = 0$$

We take into account that

$$\frac{1}{\cosh^2 \beta(h_0 + H)} = 1 - \tanh^2 \beta(h_0 + H) = 1 - \frac{h_0^2}{J^2}$$

and find

$$\partial_H h_0 = -\frac{(h_0^2 - J^2)\beta}{J + (h_0^2 - J^2)\beta}$$

Substituting this now into the expression for the magnetization we get

$$m = \frac{h_0}{J}$$