Lösungen zum Übungsblatt 6

Johannes Dörr — Übungsgruppe 2, Jürgen Lampe

Problem 1: Spin Chain

Introduction

Here, we consider a chain of spins as a model of a ferromagnet. The chain consists of $N+1$ Ising spins $s_i \in \{-1,\ 1\}$ with the Hamiltonian:

$$H(s) = -J \sum_{i=0}^{N-1} s_i s_{i+1} - B \sum_{i=0}^{N} s_i \quad , \tag{1}$$

where $J > 0$ is a constant and B an external field, that will be ignored ($B = 0$) in the following. The product $s_i s_{i+1}$ is named the i-th bond and called broken if $s_i \neq s_{i+1}$. In our case we let the $N+1$-th spin be fixed at $s_N = 1$.

Tasks

a) We give three different spin configurations (in the following also called the state of the system) for $N = 10$ and look at the resulting bond configurations.

b) The amout of states with G broken bonds is estimated.

c) We compute the energie $H(s)$ of a state s, that has $G(s)$ broken bonds.

d) A formula for the number of states with the given Energy is derived.

e) We calculate the specific entropy in the thermodynamic limit, that is:

$$s(\varepsilon) = \lim_{N\to\infty} \frac{k_B}{N} \log \Omega(\varepsilon N) \quad . \tag{2}$$

Find the temperature

$$T(\varepsilon)^{-1} = \frac{\partial s(\varepsilon)}{\partial \varepsilon} \tag{3}$$

and derive the specificenergy $\varepsilon(T)$. Compute the specific heat

$$c(T) = \frac{\partial \varepsilon(T)}{\partial T} \tag{4}$$

and plot $\varepsilon(T)$ and $c(T)$ for $k_B = 1$, $J = 1$.

Methods

a) This one is very simple as we only have to draw arrows remembering that the last spin has a defined state.

b) The amout of states including G broken bonds can be computed using a binomical coefficient, since this is a problem of combinatorics.

c) To obtain the energy we use the given Hamiltonian (eq. 1).

d) With the results of the previous items, this is a simple task.

e) To compute the specific entropy $s(\varepsilon)$ we have to calculate a binomial coefficient $\binom{N}{aN}$. For large N and $|a| < 1$ the Stirling-formula ist valid. It is used to calculate factorials approximatively:

$$N! \approx N^N e^{-N} \quad .$$

Besides that, only basic differentiations and logarithms rules are used.

Results

a) The following are three different spin configurations for $N = 10$. Faultless bonds are represented by lines ($-$) and broken bonds by dotted lines ($\cdots$).

$$\begin{gathered}
\uparrow - \uparrow - \uparrow - \uparrow \cdots \downarrow \cdots \uparrow - \uparrow \cdots \downarrow - \downarrow - \downarrow \cdots \uparrow \\
\downarrow - \downarrow - \downarrow - \cdots \uparrow - \uparrow - \uparrow \cdots \downarrow - \downarrow \cdots \uparrow - \uparrow - \uparrow \\
\downarrow - \downarrow - \downarrow - \downarrow - \downarrow - \downarrow \cdots \uparrow - \uparrow - \uparrow - \uparrow - \uparrow
\end{gathered}$$

In general, toggling all spin states obviously leads to the same sequence of broken/unbroken bonds, so there are always two corresponding spin configurations for one bond configuration.

Since the last spin is invariant in our case, its forbidden to toggle all spins. Accordingly, there is only one spin configuration.

b) The number n of states with G broken bonds is given by:

$$n = \binom{N}{G} \quad , \tag{5}$$

where $N + 1$ is the amount of spins and therefore N the number of bonds between them. See appendix for an explaination with the urn model.

c) The energy $E(s)$ of a state s with $G(s)$ broken bonds is given by:

$$E(s) = 2JG(s) - JN \quad , \tag{6}$$

with N as above.

d) The number $\Omega(E)$ of states of a given energy E can be derived from the previous results, as shown in the appendix. We obtain:

$$\Omega(E) = \binom{N}{\frac{E}{2J} + \frac{N}{2}} \quad . \tag{7}$$

e) The specific entropy $s(\varepsilon)$ is

$$s(\varepsilon) = k_B \log \left(\frac{(1-a)^a a^{-a}}{1-a} \right)$$

with $a(\varepsilon) = \left(\frac{\varepsilon}{2J} + \frac{1}{2}\right)$.
From this it follows for the temperature

$$T^{-1}(\varepsilon) = -\frac{k_B}{2J} \log \left(\frac{1 + \varepsilon/J}{1 - \varepsilon/J} \right)$$

and for the specific heat:

$$c(T) = \frac{J^2}{T^2 k_B} \left[1 - \tanh^2 \left(\frac{J}{T k_b} \right) \right] \quad .$$

For $k_B = J = 1$ the plots of $c(T)$ and $\varepsilon(T)$ (eq. 9) can be concidered in (fig. 1) and (fig. 2).

Discussion

If you take a look at (fig. 1), you'll see, that only for negative temperatures T the specific energy $\varepsilon(T)$ has positive values. This may seem implausible at first view, but isn't impossible because spin systems can have negative temperatures.

Appendix

b) We regard an urn with N numbered balls. After drawing one ball at random, let its number represent the position of a broken bond. As the binomial coefficient indicates how many possibilities there are to draw G balls out of N, it is the same as the amount of configurations with G broken bonds.

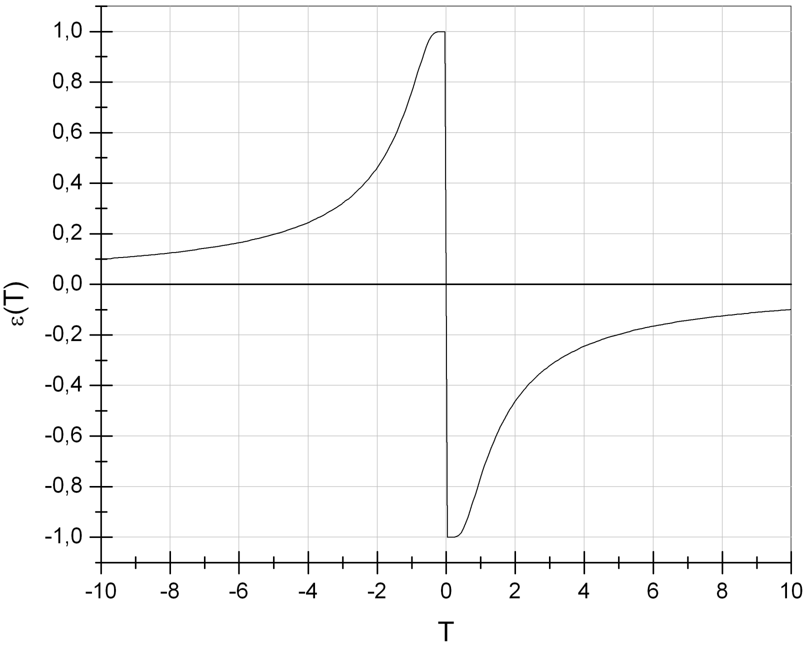

Figure 1: This plot shows the dependence of the specific energy and the temperature $\varepsilon(T)$

c) The Hamiltonian (eq. 1) specifies the energy of the state because we ignore external fields. If the i-th bond is broken, the term $s_i s_{i+1}$ is -1. Else it is 1. There are G broken and $(N-G)$ unbroken bonds, so we obtain:

$$E(s) = -J \sum_{i=0}^{N-1} s_i s_{i+1} = -J\ [N - G(s) - G(s)] = 2JG(s) - JN \quad .$$

d) The expression for the energy $E(s)$ (eq. 6) can be transformed to:

$$G(E(s)) = \frac{E}{2J} + \frac{N}{2} \quad , \tag{8}$$

so we have the number of broken bonds that result in the given energy $E(s)$. Since we are interested in the amout of states we use (eq. 5) and set in the number of broken bonds given by (eq. 8):

$$\Omega(E) = \binom{N}{\frac{E}{2J} + \frac{N}{2}} \quad .$$

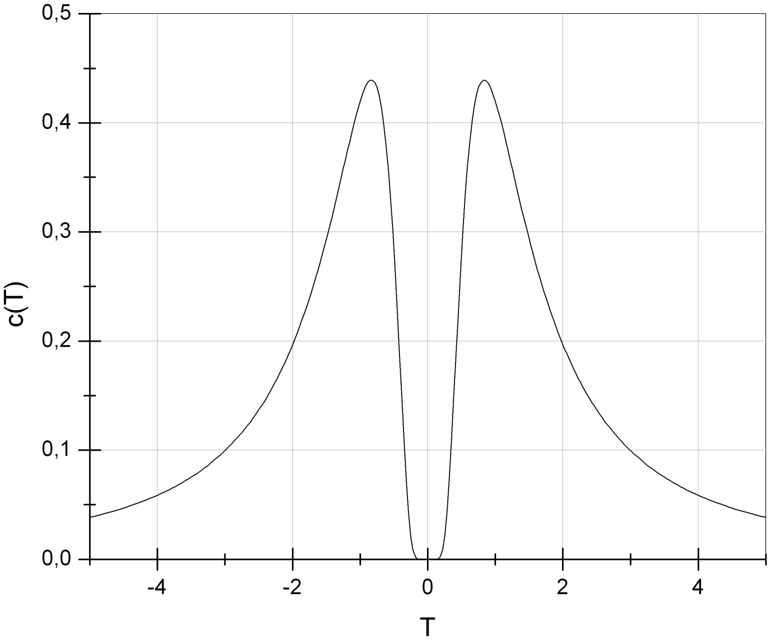

Figure 2: This plot shows the dependence of the specific heat and the temperature $c(T)$

e) Take the definition of the specific entropy (2) and the result of task 1d):

$$\begin{aligned}\Omega(E) &= \binom{N}{\frac{E}{2J}+\frac{N}{2}}\\ \Rightarrow \Omega(\varepsilon N) &= \binom{N}{N\underbrace{\left(\frac{\varepsilon}{2J}+\frac{1}{2}\right)}_{=:a}}\\ &= \binom{N}{aN}\end{aligned}$$

Insertion in (2) gives us (to approximate the factorials for large N we use the STIR-

LING-formula described in Methods):

$$\begin{aligned}
s(\varepsilon) &= \lim_{N\to\infty} \frac{k_B}{N} \log \Omega(\varepsilon N) \\
&= \lim_{N\to\infty} \frac{k_B}{N} \log \binom{N}{aN} \\
&= \lim_{N\to\infty} \frac{k_B}{N} \log \left[\frac{N!}{(N-aN)!(aN)!} \right] \\
&= \lim_{N\to\infty} \frac{k_B}{N} \log \left[\frac{N^N e^{-N}}{(N-aN)^{N-aN} e^{aN-N} (aN)^{aN} e^{-aN}} \right] \\
&= \lim_{N\to\infty} \frac{k_B}{N} \log \left[\frac{N^N}{N^N (1-a)^{N-aN} N^{-aN} a^{aN} N^{aN}} \right] \\
&= \lim_{N\to\infty} \frac{k_B}{N} \log \left[a^{-aN} (1-a)^{aN-N} \right] \\
&= \lim_{N\to\infty} \frac{k_B}{N} \left[-aN \log(a) + aN \log(1-a) - N \log(1-a) \right] \\
&= k_B \left(a \log\left(\frac{1-a}{a} \right) - \log(1-a) \right) \\
&= k_B \log\left(\frac{(1-a)^a a^{-a}}{1-a} \right)
\end{aligned}$$

We know, that $a = a(\varepsilon)$. Now we want to compute the temperature $T(\varepsilon)$:

$$\begin{aligned}
T^{-1}(\varepsilon) &= \frac{\partial s(\varepsilon)}{\partial \varepsilon} \\
&= \frac{k_B}{2J} \left(\log\left(\frac{J-\varepsilon}{J} \right) - \log\left(\frac{J+\varepsilon}{J} \right) \right) \\
&= -\frac{k_B}{2J} \left(\log\left(\frac{J+\varepsilon}{J} \right) - \log\left(\frac{J-\varepsilon}{J} \right) \right) \\
&= -\frac{k_B}{2J} \log\left(\frac{J+\varepsilon}{J-\varepsilon} \right) \\
&= -\frac{k_B}{2J} \log\left(\frac{1+\varepsilon/J}{1-\varepsilon/J} \right)
\end{aligned}$$

With hint 2 on the worksheet we get:

$$\begin{aligned}
T^{-1}(\varepsilon) &= -\frac{k_B}{J} \operatorname{artanh}\left(\frac{\varepsilon}{J} \right) \\
\Rightarrow \varepsilon(T) &= -J \tanh\left(\frac{J}{T k_B} \right) \qquad (9)
\end{aligned}$$

$\varepsilon(T)$ is the specific energy. The specific heat defined by (4) is:

$$\begin{aligned} c(T) &= \frac{\partial \varepsilon(T)}{\partial T} \\ &= \frac{J^2}{T^2 k_B} \left[1 - \tanh^2 \left(\frac{J}{T k_b} \right) \right] \end{aligned} \tag{10}$$