

## 10 Task Theoretical Physics VI - Statistics

### 10.1 (Ising model in the mean field approximation)

Spins are assigned to sites of a lattice, with the hamiltonian

$$\hat{H} = -J \sum_{\langle i,j \rangle=1}^N \hat{S}_i \hat{S}_j - \mu B \sum_{i=1}^N \hat{S}_i$$

with  $J$  the interaction strength and  $B$  an external magnetic field.

The spin operators  $\hat{S}_{i,j}$  have eigenvalues  $\pm 1$ . Using the mean field approximation the hamiltonian reduces to

$$\hat{H} = - \sum_{i=1}^N E(J, B) \hat{S}_i \text{ with } E(J, B) = \frac{1}{2} J \nu \langle \hat{S} \rangle + \mu B$$

while  $\nu$  is the number of nearest neighbors. The magnetization  $M$  is defined by:

$$M = \sum_{i=1}^N \mu_i \langle \hat{S}_i \rangle = N \mu \langle \hat{S} \rangle \quad (1)$$

(a)

While we already treated a two state system in task 7.4 this problem has just to be rewritten into n-particle form.

Definition partition function:

$$Z = \text{Tr} \left( e^{-\beta \hat{H}} \right)$$

inserting the hamiltonian:

$$\begin{aligned} Z &= \text{Tr} \left( e^{\beta \sum_{i=1}^N E(J, B) \hat{S}_i} \right) \\ &= \text{Tr} \left( \prod_{i=1}^N e^{\beta E \hat{S}_i} \right) \\ &= \sum_{S_1, \dots, S_N} \prod_{i=1}^N \langle \psi | e^{\beta E \hat{S}_i} | \psi \rangle \\ &= \sum_{S_1, \dots, S_N} \prod_{i=1}^N \langle S_1 | \dots | S_N | e^{\beta E \hat{S}_i} | S_1 \rangle \dots | S_N \rangle \end{aligned}$$

while we got two states for each particle  $S_i = \pm$  this leads to:

$$\begin{aligned} Z &= \prod_{i=1}^N (e^{\beta E} + e^{-\beta E}) \\ &= \prod_{i=1}^N 2 \cosh \beta E \\ &= (2 \cosh \beta E)^N \end{aligned}$$

Definition of specific gibbs free energy:

$$g(J, B) = f(J, B) - Bm$$

while the term  $Ts$  can be rewritten here to  $Bm$  because of the model of ferromagnetism which is observed. The regularity can be measured using the magnetisation  $m$ , while the external magneticfield  $B$  will change it. With

$$f = -\frac{1}{\beta} \ln Z$$

we get:

$$g = -\frac{N}{\beta} \ln (2 \cosh \beta E) - Bm$$

We are meant to show that:

$$\langle \hat{\mathbf{S}} \rangle = \tanh \left( \langle \hat{\mathbf{S}} \rangle \frac{T_c}{T} + \beta \mu B \right) \quad \text{with} \quad T_c = \frac{\nu J}{2k_B} \quad (2)$$

This can be done easily (we use  $\hat{\mathbf{S}} = \frac{1}{N} \sum_{i=1}^N \hat{\mathbf{S}}_i \Leftrightarrow \sum_{i=1}^N \hat{\mathbf{S}}_i = N\hat{\mathbf{S}}$ ):

$$\begin{aligned} \langle \hat{\mathbf{S}} \rangle &= \frac{1}{Z} \text{Tr} \left( e^{-\beta H \hat{\mathbf{S}}} \right) \\ &= \frac{1}{Z} \text{Tr} \left( e^{-\beta EN \hat{\mathbf{S}}} \right) \\ &= -\frac{1}{Z} \frac{\partial}{\partial (\beta EN)} \text{Tr} \left( e^{-\beta EN \hat{\mathbf{S}}} \right) \\ &= \frac{1}{ZEN} \frac{\partial}{\partial \beta} Z \\ &= \frac{1}{ZEN} \frac{\partial}{\partial \beta} (2 \cosh \beta E)^N \\ &= \frac{1}{ZEN} \left( N \cdot (2 \cosh \beta E)^{N-1} \cdot 2 \sinh \beta E \cdot E \right) \\ &= \frac{(2 \cosh \beta E)^N \sinh \beta E}{Z \cosh \beta E} \\ &= \tanh \beta E \\ &= \tanh \left( \langle \hat{\mathbf{S}} \rangle \frac{J\nu}{2k_B T} + \beta \mu B \right) \\ &= \tanh \left( \langle \hat{\mathbf{S}} \rangle \frac{T_c}{T} + \beta \mu B \right) \end{aligned}$$

□

(b)

We now want to intepret equation (2) geometrically for  $B = 0$ :

$$\langle \hat{\mathbf{S}} \rangle = \tanh \left( \langle \hat{\mathbf{S}} \rangle \frac{T_c}{T} \right) \quad (3)$$

therefore we got two dependences, while we think of  $T_c$  being a constant, we can vary the temperature (or the factor  $T_c/T$ ) and theoretically  $\langle \hat{\mathbf{S}} \rangle$  can be varied, too. We first plot (in fig. (1)) both sides in a diagram, while the left side is the red plot and the right side is represented by the black plots, while  $T_c/T$  is varied.

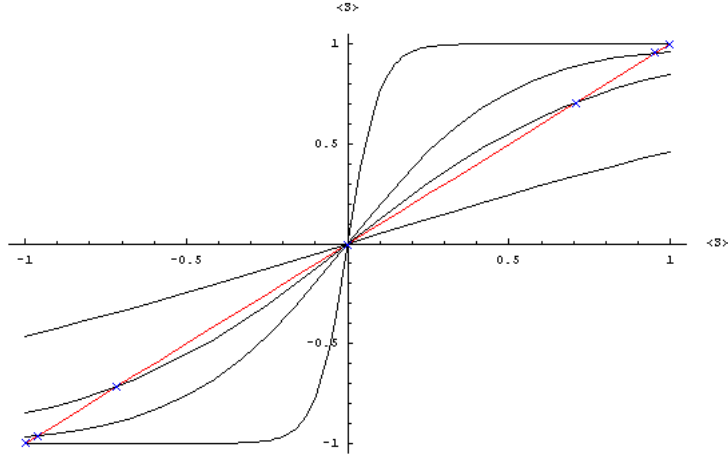


Figure 1: Plot of right and left hand side of equation (3), while the intercepts are marked with a blue cross.

From this plot we can learn, that for  $T_c/T < 1 \Leftrightarrow T_c < T$  there will only be the solution  $\langle \hat{\mathbf{S}} \rangle = 0$ , while for  $T < T_c$  we have three solutions  $\langle \hat{\mathbf{S}} \rangle = 0, \pm S_0(T)$ , while  $S_0(T)$  is depending on the temperature. A physical interpretation might be that the two possible non-zero values for  $\langle \hat{\mathbf{S}} \rangle$  in the case of  $T < T_c$  represent two cases of ordering the spins on that temperature, while an external field isn't needed. For the case  $T > T_c$  there will always be the need of an external field to order the spins. But having  $\langle \hat{\mathbf{S}} \rangle \neq 0$  means we have a magnetization. This means above  $T_c$ , which now can be identified as the Curie temperature, there will be no ferromagnetism anymore.

(c)

We are now looking at the two special cases  $T \approx 0$  K and  $T \approx T_c$ , while  $B = 0$ . We start out using equation (3):

$$\begin{aligned}
\langle \hat{\mathbf{S}} \rangle &= \tanh\left(\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) \\
\langle \hat{\mathbf{S}} \rangle \cosh\left(\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) &= \sinh\left(\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) \\
\langle \hat{\mathbf{S}} \rangle \left(\exp\left(\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) + \exp\left(-\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right)\right) &= \exp\left(\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) - \exp\left(-\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) \\
\langle \hat{\mathbf{S}} \rangle \left(\exp\left(2\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) + 1\right) &= \exp\left(2\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) - 1 \\
\exp\left(2\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) (\langle \hat{\mathbf{S}} \rangle - 1) &= -(\langle \hat{\mathbf{S}} \rangle + 1)
\end{aligned}$$

Now using  $T \approx 0 \text{ K}$  we can use, that  $\lim_{x \rightarrow \infty} \tanh x \approx 1$  therefore  $\langle \hat{\mathbf{S}} \rangle \approx 1$ , which leads to:

$$\begin{aligned}
\langle \hat{\mathbf{S}} \rangle - 1 &= -2 \exp\left(-2\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) \\
\langle \hat{\mathbf{S}} \rangle &= 1 - 2 \exp\left(-2\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right)
\end{aligned}$$

□

For  $T \approx T_c$  we can evaluate the tanh-function:

$$\tanh\left(\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) \approx \langle \hat{\mathbf{S}} \rangle \frac{T_c}{T} - \frac{1}{3} \left(\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right)^3 + \mathcal{O}\left(\frac{2}{15} \left(\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right)^5\right)$$

inserting in (3) leads to:

$$\begin{aligned}
\langle \hat{\mathbf{S}} \rangle &= \tanh\left(\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right) \\
\langle \hat{\mathbf{S}} \rangle &= \langle \hat{\mathbf{S}} \rangle \frac{T_c}{T} - \frac{1}{3} \left(\langle \hat{\mathbf{S}} \rangle \frac{T_c}{T}\right)^3 \\
\langle \hat{\mathbf{S}} \rangle^2 &= \left(\frac{T}{T_c}\right)^3 3 \left(\frac{T_c}{T} - 1\right) \\
\langle \hat{\mathbf{S}} \rangle &= \frac{T}{T_c} \sqrt{3 \left(1 - \frac{T}{T_c}\right)} \tag{4}
\end{aligned}$$

now the prefactor  $\frac{T}{T_c} \approx 1$ , we get:

$$\langle \hat{\mathbf{S}} \rangle \approx \sqrt{3 \left(1 - \frac{T}{T_c}\right)}$$

□

(d)

With definition of heat capacity:

$$C = \frac{\partial U}{\partial T}$$

and the inner energy (using  $\sum_{i=1}^N = N\hat{\mathbf{S}}$ )

$$U = \langle \hat{\mathbf{H}} \rangle = \left\langle - \sum_{i=1}^N E(J, B) \hat{\mathbf{S}}_i \right\rangle = \left\langle - \sum_{i=1}^N \left( \frac{1}{2} J\nu \langle \hat{\mathbf{S}} \rangle + \mu B \right) \hat{\mathbf{S}}_i \right\rangle = -\frac{1}{2} J\nu N \langle \hat{\mathbf{S}} \rangle^2 + N\mu B \langle \hat{\mathbf{S}} \rangle$$

we get:

$$\begin{aligned} C &= \frac{\partial}{\partial T} \left( -\frac{1}{2} J\nu N \langle \hat{\mathbf{S}} \rangle^2 + N\mu B \langle \hat{\mathbf{S}} \rangle \right) \\ &= -J\nu N \langle \hat{\mathbf{S}} \rangle \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial T} + N\mu B \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial T} \end{aligned}$$

we now want to find a solution for  $\frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial T}$ , which we try to find by inserting equation (2).

$$\frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial T} = \frac{\partial}{\partial T} \tanh \left( \langle \hat{\mathbf{S}}(T) \rangle \frac{T_c}{T} + \frac{\mu B}{k_B T} \right)$$

using *mathematica* to solve this differentiation we get:

$$\frac{\partial}{\partial T} \tanh \left( \langle \hat{\mathbf{S}}(T) \rangle \frac{T_c}{T} + \frac{\mu B}{k_B T} \right) = \frac{\left( \frac{T_c}{T} \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial T} - \frac{\mu B}{k_B T^2} - \frac{T_c \langle \hat{\mathbf{S}} \rangle}{T^2} \right)}{\left( \cosh \left( \langle \hat{\mathbf{S}}(T) \rangle \frac{T_c}{T} + \frac{\mu B}{k_B T} \right) \right)^2}$$

using  $(\cosh(x))^2 = 1 - (\tanh(x))^2$  and equation (2) leads to:

$$\frac{\partial}{\partial T} \tanh \left( \langle \hat{\mathbf{S}}(T) \rangle \frac{T_c}{T} + \frac{\mu B}{k_B T} \right) = \frac{\left( \frac{T_c}{T} \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial T} - \frac{\mu B}{k_B T^2} - \frac{T_c \langle \hat{\mathbf{S}} \rangle}{T^2} \right)}{1 - \langle \hat{\mathbf{S}} \rangle^2}$$

inserting this

$$\frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial T} = \frac{\mu B + k_B T_c \langle \hat{\mathbf{S}} \rangle}{k_B T^2 \left[ \langle \hat{\mathbf{S}} \rangle^2 - 1 + \frac{T_c}{T} \right]}$$

which can be reinserted and this leads to:

$$\begin{aligned}
C &= -J\nu N \langle \hat{\mathbf{S}} \rangle \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial T} + N\mu B \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial T} \\
&= \frac{N \left( \mu B + k_B T_c \langle \hat{\mathbf{S}} \rangle \right)}{k_B T^2 \left[ \langle \hat{\mathbf{S}} \rangle^2 - 1 + \frac{T_c}{T} \right]} \left( -J\nu \langle \hat{\mathbf{S}} \rangle + \mu B \right)
\end{aligned}$$

to calculate the jump at  $T = T_c$  we can use, that  $\langle \hat{\mathbf{S}} \rangle = 0$  for  $T > T_c$ , meaning we have:

$$\lim_{T \searrow T_c} C = \frac{N(\mu B)^2}{k_B T [T_c - T]}$$

for  $B = 0$  we get:

$$\lim_{T \searrow T_c} C = 0$$

For  $T \approx T_c$  we can use the approximation from equation (4), while we now have to say  $B = 0$ :

$$\begin{aligned}
\lim_{T \nearrow T_c} C &= \frac{N \left( \mu B + k_B T \sqrt{3 \left( 1 - \frac{T}{T_c} \right)} \right) \left( -J\nu \frac{T}{T_c} \sqrt{3 \left( 1 - \frac{T}{T_c} \right)} + \mu B \right)}{k_B T^2 \left[ 3 \frac{T^2}{T_c^2} \left( 1 - \frac{T}{T_c} \right) - 1 + \frac{T_c}{T} \right]} \\
&= \frac{N \left( (\mu B)^2 - \mu B J\nu \frac{T}{T_c} \sqrt{3 \left( 1 - \frac{T}{T_c} \right)} + \mu B k_B T \sqrt{3 \left( 1 - \frac{T}{T_c} \right)} - 3J\nu k_B \frac{T^2}{T_c} \left( 1 - \frac{T}{T_c} \right) \right)}{k_B T^2 \left[ 3 \frac{T^2}{T_c^2} \left( 1 - \frac{T}{T_c} \right) - \left( 1 - \frac{T_c}{T} \right) \right]} \\
&= \frac{N \left( (\mu B)^2 - \mu B J\nu \frac{T}{T_c} \sqrt{3 \left( 1 - \frac{T}{T_c} \right)} + \mu B k_B T \sqrt{3 \left( 1 - \frac{T}{T_c} \right)} \right)}{k_B \frac{T^2}{T_c} \left[ \left( 3 \frac{T^2}{T_c^2} - 1 \right) (T_c - T) \right]} - \frac{3NJ\nu}{T_c \left( 3 \frac{T^2}{T_c^2} - 1 \right)}
\end{aligned}$$

Now we can use, that  $T \approx T_c$ , this leads to:

$$\begin{aligned}
\lim_{T \nearrow T_c} C &= \frac{N(\mu B)^2}{2k_B T (T_c - T)} - \frac{3NJ\nu}{2T_c} \\
&= \frac{N(\mu B)^2}{2k_B \frac{T^2}{T_c} (T_c - T)} - 3Nk_B
\end{aligned}$$

while we used the approximation we have to use  $B = 0$ :

$$\lim_{T \nearrow T_c} C = -3Nk_B$$

Therefore comparing  $\lim_{T \nearrow T_c} C$  and  $\lim_{T \searrow T_c} C$  (for  $B = 0$ ) leads to the jump of:

$$\Delta C \Big|_{T=T_c} = 3Nk_B$$

This means we got a gap of  $3Nk_B$  at the Curie temperature, if there is no external field  $B$ . If we have an external field  $B$  it seems to become some kind of more complicated, while the approximation we used needs to be modified, which seems to be quite a hard task of work.

(e)

We now have to calculate the magnetic susceptibility

$$\chi_{T,N}(B=0) = \frac{\partial M}{\partial B} \Big|_{T,N}$$

for  $T \approx T_c$  with  $\lim_{T \nearrow T_c}$  and  $\lim_{T \searrow T_c}$ . We use equation (1):

$$M = N\mu \langle \hat{\mathbf{S}} \rangle$$

to get:

$$\frac{\partial M}{\partial B} = N\mu \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial B}$$

inserting equation (2) leads to:

$$\frac{\partial M}{\partial B} = N\mu \frac{\partial}{\partial B} \tanh \left( \langle \hat{\mathbf{S}}(B) \rangle \frac{T_c}{T} + \beta\mu B \right)$$

where we have to differentiate:

$$\begin{aligned} \frac{\partial}{\partial B} \tanh \left( \langle \hat{\mathbf{S}}(B) \rangle \frac{T_c}{T} + \beta\mu B \right) &= \frac{\left( \frac{\mu}{k_B T} + \frac{T_c}{T} \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial B} \right)}{\left( \cosh \left( \langle \hat{\mathbf{S}}(B) \rangle \frac{T_c}{T} + \frac{\mu B}{k_B T} \right) \right)^2} \\ &= \frac{\left( \frac{\mu}{k_B T} + \frac{T_c}{T} \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial B} \right)}{1 - \langle \hat{\mathbf{S}} \rangle^2} \end{aligned}$$

This leads to:

$$\begin{aligned} \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial B} &= \frac{\left( \frac{\mu}{k_B T} + \frac{T_c}{T} \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial B} \right)}{1 - \langle \hat{\mathbf{S}} \rangle^2} \\ \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial B} &= \frac{\mu}{k_B T \left( 1 - \langle \hat{\mathbf{S}} \rangle^2 - \frac{T_c}{T} \right)} \end{aligned}$$

now we can insert it

$$\begin{aligned}\frac{\partial M}{\partial B} &= N\mu \frac{\partial \langle \hat{\mathbf{S}} \rangle}{\partial B} \\ &= \frac{N\mu^2}{k_B T \left( 1 - \langle \hat{\mathbf{S}} \rangle^2 - \frac{T_c}{T} \right)}\end{aligned}$$

We again want to use our approximation from equation (4), which can be used for  $T < T_c$  and  $B = 0$ :

$$\begin{aligned}\frac{\partial M}{\partial B} &= \frac{N\mu^2}{k_B T \left( 1 - 3\frac{T^2}{T_c^2} \left( 1 - \frac{T}{T_c} \right) - \frac{T_c}{T} \right)} \\ \chi_{T,N}(B=0) &= \frac{N\mu^2}{k_B T \left( 1 - 3\frac{T^2}{T_c^2} \left( 1 - \frac{T}{T_c} \right) - \frac{T_c}{T} \right)} \\ \chi_{T,N}(B=0) &= \frac{N\mu^2}{k_B \frac{T}{T_c^3} (T_c^3 - 3T^3)}\end{aligned}$$

if we use  $\frac{T}{T_c} \approx \frac{T^2}{T_c^2} \approx 1$ , which will be nearer to 1 for  $T < T_c$  and  $T \approx T_c$  as the cubic term. Now we try the next approximation with  $\langle \hat{\mathbf{S}} \rangle^2 = 0$  while  $T > T_c$  and  $B = 0$ , we get:

$$\chi_{T,N}(B=0) = \frac{N\mu^2}{k_B (T - T_c)}$$

This is the famous Curie-Weiss-Law

$$\chi_m = \frac{C}{T - T_c}$$

with  $C = \frac{N\mu^2}{k_B}$ . But while the first result seems some kind of unlikely we seem to need another method of resolution. We try to evaluate (first order) equation (2) while for  $T \approx T_c$  it will be small

$$\begin{aligned}\langle \hat{\mathbf{S}} \rangle &= \langle \hat{\mathbf{S}} \rangle \frac{T_c}{T} + \beta\mu B \\ M &= \frac{N\mu^2 B}{k_B (T - T_c)}\end{aligned}$$

therefore we get the susceptibility:

$$\chi = \frac{N\mu^2}{k_B (T - T_c)}$$

which we already had and which is Curie-Weiss-law again. To get a dependence of the side we come from with  $T$  to  $T_c$  we are going further one order in the evaluation:



$$\begin{aligned}
\langle \hat{\mathbf{S}} \rangle &= \langle \hat{\mathbf{S}} \rangle \frac{T_c}{T} + \beta \mu B - \frac{1}{3} \left( \langle \hat{\mathbf{S}} \rangle \frac{T_c}{T} + \beta \mu B \right)^3 \\
(T - T_c) \langle \hat{\mathbf{S}} \rangle &= \frac{\mu B}{k_B} - \frac{1}{3T^2} \left( \langle \hat{\mathbf{S}} \rangle T_c + \frac{\mu B}{k_B} \right)^3 \\
(T - T_c) \langle \hat{\mathbf{S}} \rangle &= \frac{\mu B}{k_B} - \frac{1}{3T^2} \left( \left( \langle \hat{\mathbf{S}} \rangle T_c \right)^3 + \langle \hat{\mathbf{S}} \rangle^2 T_c \frac{\mu B}{k_B} + \langle \hat{\mathbf{S}} \rangle T_c \left( \frac{\mu B}{k_B} \right)^2 + \left( \frac{\mu B}{k_B} \right)^3 \right)
\end{aligned}$$

while it is easy to see, that this term will become quite a beast to handle, we will use the approximation, that  $B$  is small therefore we will cancel the  $B^2$  and the  $B^3$  term leading to:

$$(T - T_c) \langle \hat{\mathbf{S}} \rangle = \frac{\mu B}{k_B} - \frac{T_c^3}{3T^2} \langle \hat{\mathbf{S}} \rangle^3 - \frac{T_c}{3T^2} \langle \hat{\mathbf{S}} \rangle^2 \frac{\mu B}{k_B}$$

now the  $\langle \hat{\mathbf{S}} \rangle^2 B$  term can be cancelled, since it will also be small because of  $\langle \hat{\mathbf{S}} \rangle^2$  being not too large and  $B$  being small. Therefore this is simplified to:

$$\frac{T_c^3}{3T^3} \langle \hat{\mathbf{S}} \rangle^3 + \frac{(T - T_c)}{T} \langle \hat{\mathbf{S}} \rangle = \frac{\mu B}{k_B T}$$

now using  $T \approx T_c$  this is:

$$\frac{1}{3} \langle \hat{\mathbf{S}} \rangle^3 + \frac{(T - T_c)}{T} \langle \hat{\mathbf{S}} \rangle = \frac{\mu B}{k_B T}$$

Now inserting  $\langle \hat{\mathbf{S}} \rangle = M / (N\mu)$  leads to:

$$\frac{1}{3} \left( \frac{M}{N\mu} \right)^3 + \frac{(T - T_c)}{T} \frac{M}{N\mu} = \frac{\mu B}{k_B T}$$

we can differentiate both sides with  $\partial/\partial B$  this leads to, using  $\chi_{T,N}(B=0) = \frac{\partial M}{\partial B}$ :

$$\frac{M^2 \chi}{(N\mu)^3} + \frac{(T - T_c)}{T} \frac{\chi}{N\mu} = \frac{\mu}{k_B T}$$

this can be rearranged to:

$$\begin{aligned}
\chi \left( \frac{M^2}{(N\mu)^3} + \frac{(T - T_c)}{N\mu T} \right) &= \frac{\mu}{k_B T} \\
\chi &= \frac{N\mu^2}{k_B \left( \langle \hat{\mathbf{S}} \rangle^2 T + (T - T_c) \right)}
\end{aligned}$$

Now one more time the approximations for  $\langle \hat{\mathbf{S}} \rangle$  can be used for  $T < T_c$  and  $T > T_c$ , which lead to:

$$\chi = \begin{cases} \frac{N\mu^2}{2k_B(T_c - T)}, & T < T_c \\ \frac{N\mu^2}{k_B(T - T_c)}, & T > T_c \end{cases}$$

one more time Curie-Weiss-law for  $T > T_c$ . But a new version for  $T < T_c$ . With the critical exponents we will see, that this one fits the expectation better, since it leads to the same critical exponent like the case  $T > T_c$ .

We now have to calculate the critical exponents. First for the case of  $T > T_c$ , definition of critical exponent:

$$\lambda = \lim_{\epsilon \rightarrow 0} \frac{\ln |f(\epsilon)|}{\ln |\epsilon|}$$

with

$$f(\epsilon) = A \left( \frac{T - T_c}{T_c} \right)^{-\lambda} = \left( \frac{N\mu^2}{k_B T_c} \right) \left( \frac{T - T_c}{T_c} \right)^{-1}$$

therefore the critical exponent is  $\lambda = 1$  and  $A = \frac{N\mu^2}{k_B T_c}$ . Now the case for  $T < T_c$ :

$$f(\epsilon) = A \left( \frac{T - T_c}{T_c} \right)^\lambda \left[ 1 + B \left( \frac{T - T_c}{T_c} \right)^y + \dots \right] = \frac{N\mu^2}{k_B \frac{T}{T_c^3} (T_c^3 - 3T^3)}$$

while the result seems to be wrong, we will not further try to find the critical exponent. But it seems likely that the result of the critical exponent will be the same with  $\lambda = 1$  for  $T < T_c$ . Meaning both critical exponents are the same. Now for the other result:

$$f(\epsilon) = A \left( \frac{T - T_c}{T_c} \right)^{-\lambda} = (-1)^\lambda \frac{N\mu^2}{2k_B T_c} \left( \frac{T - T_c}{T_c} \right)^{-1}$$

this means the critical exponent is indeed the same  $\lambda = 1$  and this time  $A = -\frac{N\mu^2}{2k_B T_c}$ .

Or we can do it alternatively with:

$$\chi = \begin{cases} -\frac{N\mu^2}{2k_B T_c \epsilon} = \frac{A_1}{\epsilon}, & T < T_c \\ \frac{N\mu^2}{k_B T_c \epsilon} = \frac{A_2}{\epsilon}, & T > T_c \end{cases}$$

while  $\epsilon = \frac{T - T_c}{T_c}$ , this leads to the critical exponents:

$$\lambda = \begin{cases} \lim_{\epsilon \rightarrow 0} \frac{\ln \left| \frac{A_1}{\epsilon} \right|}{\ln |\epsilon|} = \lim_{\epsilon \rightarrow 0} \left| \frac{\ln A_1}{\ln \epsilon} - \frac{\ln \epsilon}{\ln \epsilon} \right| = 1, & T < T_c \\ \lim_{\epsilon \rightarrow 0} \frac{\ln \left| \frac{A_2}{\epsilon} \right|}{\ln |\epsilon|} = 1 & T > T_c \end{cases}$$

## 10.2 (Correct counting statistics)

System of three particles and three single particle energy levels  $E_i = 0, \epsilon, 2\epsilon$ . We will calculate the partition functions for:

**(a) bosons**

We first do it explicitly using the characteristics of bosons, meaning, they can all occupy the same energy state:

0	$\epsilon$	$2\epsilon$	$\epsilon_{tot}$
3	0	0	0
2	1	0	1
2	0	1	2
1	1	1	3
1	2	0	2
1	0	2	4
0	3	0	3
0	2	1	4
0	1	2	5
0	0	3	6

This means, we got 10 different states. This is the same problem like task 7.1 meaning the number of states is defined with:

$$Z_{N_i}(N) = \binom{N + N_i - 1}{N_i} = \frac{(N + N_i - 1)!}{N_i!(N - 1)!}$$

while  $N$  is the number of single-particle energy states and  $N_i$  is the number of quanta, meaning:

$$Z_3(3) = \binom{3 + 3 - 1}{3} = \frac{5!}{3!2!} = 10$$

the formula has already been proven in task 7.1 using induction. Alternatively we can write the partition function using:

$$\begin{aligned} Z &= \text{Tr}e^{-\beta\hat{H}} \\ &= \sum_{i=1}^{10} e^{-\beta E_i} \\ &= 1 + e^{-\beta\epsilon} + 2e^{-2\beta\epsilon} + 2e^{-3\beta\epsilon} + 2e^{-4\beta\epsilon} + e^{-5\beta\epsilon} + e^{-6\beta\epsilon} \end{aligned}$$

**(b) spin-polarized fermions**

Again explicitly first, while we have spin-polarized fermions, there is the pauli-principle which doesn't allow two particles to be in the same state. This means:

0	$\epsilon$	$2\epsilon$	$\epsilon_{tot}$
1	1	1	3

as the only possibility, therefore the result is:

$$Z_3(3) = 1$$

to derive a formula for this, we already know, that for the same amount of energy states and particles we will always get only one possible state. Now we will consider the case of  $n$  particles and  $M$  single-particle energystates, first for an example  $n = 1, M = 2$ , meaning

$\epsilon_1$	$\epsilon_2$
1	0
0	1

meaning  $Z_n(M) = Z_1(2) = 2$ . for  $n = 1, M = 3$  it is  $Z_1(3) = 3$ . Now using  $n = 2, M = 3$  we get

$\epsilon_1$	$\epsilon_2$	$\epsilon_3$
1	1	0
1	0	1
0	1	1

leading to  $Z_2(3) = 3$ . At last  $n = 2, M = 4$ , with

$\epsilon_1$	$\epsilon_2$	$\epsilon_3$	$\epsilon_4$
1	1	0	0
1	0	1	0
1	0	0	1
0	1	1	0
0	1	0	1
0	0	1	1

we have  $Z_2(4) = 6$ . Therefore we can have a look at our bordering conditions,

$$\begin{aligned} Z_1(M) &= M \\ Z_n(M) &= 1, \text{ for } n = M \end{aligned}$$

to guess a partition function:

$$Z_n(M) = \binom{M}{n} = \frac{M!}{n!(M-n)!}$$

for our examples this leads to:

$$Z_1(2) = \frac{2!}{1!(2-1)!} = 2$$

$$Z_1(3) = \frac{3!}{1!(3-1)!} = 3$$

$$Z_2(3) = \frac{3!}{2!(3-2)!} = 3$$

$$Z_3(3) = \frac{3!}{3!(3-3)!} = 1$$

$$Z_2(4) = \frac{4!}{2!(4-2)!} = 6$$

Induction:

$$Z_1(M) = \binom{M}{1} = \frac{M!}{1!(M-1)!} = \frac{M \cdot (M-1)!}{(M-1)!} = M$$

now  $M \rightarrow M + 1$ :

$$\begin{aligned} Z_1(M+1) &= \binom{M+1}{1} \\ &= \frac{(M+1)!}{1!M!} \\ &= \frac{(M+1)M!}{M!} \\ &= M+1 \end{aligned}$$

and the second bordering condition is fulfilled proven by induction:

$$Z_1(1) = \binom{1}{1} = \frac{1!}{1!(1-1)!} = 1$$

and  $n \rightarrow n + 1, M \rightarrow M + 1$  for  $n = M$ :

$$\begin{aligned} Z_{n+1}(n+1) &= \binom{n+1}{n+1} \\ &= \frac{(n+1)!}{(n+1)!(n+1-n-1)!} \\ &= 1 \end{aligned}$$

Therefore our partition function is:

$$Z_n(M) = \binom{M}{n} = \frac{M!}{n!(M-n)!}$$

and for the special case  $n = 3, M = 3$  this leads to:

$$Z_3(3) = 1$$

Alternatively again for the partition function:

$$Z = e^{-3\beta\epsilon}$$

### (c) distinguishable particles

We again start out counting explicitly, while the particles are distinguishable, we can give a label to them, labeling them a, b and c:

0	$\epsilon$	$2\epsilon$	$\epsilon_{tot}$
abc	0	0	0
ab	c	0	1
ab	0	c	2
ac	b	0	1
ac	0	b	2
bc	a	0	1
bc	0	a	2
a	bc	0	2
a	0	bc	4
a	b	c	3
a	c	b	3
b	ac	0	2
b	0	ac	4
b	a	c	3
b	c	a	3
c	ab	0	2
c	0	ab	4
c	a	b	3
c	b	a	3
0	abc	0	3
0	ab	c	4
0	ac	b	4
0	bc	a	4
0	a	bc	5
0	b	ac	5
0	c	ab	5
0	0	abc	6

This means

$$Z_3(3) = 27 = 3^3$$

now we want to get the formula to calculate it. Starting with examples, while it can be immediately seen, that

$$Z_1(M) = M = M^1$$

holds. This means,  $n = 1$  is already well known, also we know:

$$Z_n(1) = 1 = 1^n$$

Now we start with examples, while we already know all possible results of the combinations of  $n = 1$  and  $M = 1$  we start with  $n = 2$ ,  $M = 2$ :

$\epsilon_1$	$\epsilon_2$
ab	0
a	b
b	a
0	ab

This means  $Z_2(2) = 4 = 2^2$ . Further:

$$\begin{aligned} Z_2(3) &= 9 = 3^2 \\ Z_3(2) &= 8 = 2^3 \end{aligned}$$

We conclude:

$$Z_n(M) = M^n$$

This means for the given problem:

$$Z_3(3) = 27$$

We alternatively get (nice “symmetry” 1, 3, 6, 7, 6, 3, 1):

$$Z = 1 + 3e^{-\beta\epsilon} + 6e^{-2\beta\epsilon} + 7e^{-3\beta\epsilon} + 6e^{-4\beta\epsilon} + 3e^{-5\beta\epsilon} + e^{-6\beta\epsilon}$$

### 10.3 (Conservation of symmetry)

The time evolution operator is defined with:

$$\hat{U}(t, t_0) = I - \frac{i}{\hbar} \int_{t_0}^t dt' \hat{\mathbf{H}}(t') \hat{U}(t', t_0)$$

with  $I$  being the identity. We are meant to show, that it commutes with any permutation operator  $\hat{\mathbf{P}}_{ij}$  for a system of identical particles. We furthermore consider  $\hat{\mathbf{H}} = \hat{\mathbf{H}}(t)$  a time-dependent hamiltonian. While the hamiltonian is explicitly time dependent the time evolution operator can be rewritten using the Dyson-series:

$$\begin{aligned} \hat{U}(t, t_0) &= I - \frac{i}{\hbar} \int_{t_0}^t dt' \hat{\mathbf{H}}(t') + \left(\frac{i}{\hbar}\right)^2 \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \hat{\mathbf{H}}(t') \hat{\mathbf{H}}(t'') \hat{U}(t'', t_0) \\ &= I + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^t dt_1 dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n \hat{\mathbf{H}}(t_1) \hat{\mathbf{H}}(t_2) \dots \hat{\mathbf{H}}(t_n) \quad (5) \end{aligned}$$

While we showed in the lecture, that the permutation operator and a given observable  $\hat{\mathbf{A}}_N$  fulfill

$$\hat{\mathbf{A}}_N = \hat{\mathbf{P}}_{ij}^\dagger \hat{\mathbf{A}}_N \hat{\mathbf{P}}_{ij}$$

which is equal to

$$\hat{\mathbf{P}}_{ij} \hat{\mathbf{A}}_N = \hat{\mathbf{A}}_N \hat{\mathbf{P}}_{ij} \Leftrightarrow \hat{\mathbf{P}}_{ij} \hat{\mathbf{A}}_N - \hat{\mathbf{A}}_N \hat{\mathbf{P}}_{ij} = 0$$

while we used  $\hat{\mathbf{P}}_{ij} \hat{\mathbf{P}}_{ij}^\dagger = \hat{\mathbf{P}}_{ij}^2 = I$ . But this means the permutation operator commutes with the observable, especially for the hamiltonian  $\hat{\mathbf{H}} = \hat{\mathbf{A}}_N$ , this means we get:

$$\left[ \hat{\mathbf{P}}_{ij}, \hat{\mathbf{H}} \right] = 0$$

Now we can insert the time evolution operator:

$$\left[ \hat{\mathbf{P}}_{ij}, \hat{\mathbf{U}}(t, t_0) \right] \stackrel{?}{=} 0$$

while we saw in equation (5), that  $\hat{\mathbf{U}}(t, t_0)$  consists only of hamiltonians and the identity, we can insert  $\hat{\mathbf{U}}(t, t_0)$ :

$$\begin{aligned} \left[ \hat{\mathbf{P}}_{ij}, \hat{\mathbf{U}}(t, t_0) \right] &= \left[ \hat{\mathbf{P}}_{ij}, I \right] + \left[ \hat{\mathbf{P}}_{ij}, \sum_{n=1}^{\infty} \left( -\frac{i}{\hbar} \right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n \hat{\mathbf{H}}(t_1) \hat{\mathbf{H}}(t_2) \dots \hat{\mathbf{H}}(t_n) \right] \\ &= 0 + \left[ \hat{\mathbf{P}}_{ij}, \sum_{n=1}^{\infty} \left( -\frac{i}{\hbar} \right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n \hat{\mathbf{H}}(t_1) \hat{\mathbf{H}}(t_2) \dots \hat{\mathbf{H}}(t_n) \right] \end{aligned}$$

while the permutation operator isn't affected by the integration and summation, we can rewrite it to:

$$\left[ \hat{\mathbf{P}}_{ij}, \hat{\mathbf{U}}(t, t_0) \right] = \sum_{n=1}^{\infty} \left( -\frac{i}{\hbar} \right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n \left[ \hat{\mathbf{P}}_{ij}, \hat{\mathbf{H}}(t_1) \hat{\mathbf{H}}(t_2) \dots \hat{\mathbf{H}}(t_n) \right]$$

Now the commutator  $\left[ \hat{\mathbf{P}}_{ij}, \hat{\mathbf{H}}(t_1) \hat{\mathbf{H}}(t_2) \dots \hat{\mathbf{H}}(t_n) \right]$  is of the form  $[A, BC \dots Z]$ , which can be split in a sum of commutators of the form  $c_1 [A, B] c_2 + c_3 [A, C] c_4 + \dots + c_{n-1} [A, Z] c_n$  (with  $c_i$  being products of operators), explicitly for the simplified case of  $n = 2$  (here  $c_1 = I$ ,  $c_2 = C$ ,  $c_3 = B$ ,  $c_4 = I$  with  $I$  the identity):

$$[A, BC] = ABC \underbrace{-BAC + BAC}_{=0} -BCA = [A, B] C + B [A, C]$$

but while  $\left[ \hat{\mathbf{P}}_{ij}, \hat{\mathbf{H}}(t_n) \right] = 0$  we only have 0's in the sum and therefore:

$$\left[ \hat{\mathbf{P}}_{ij}, \hat{\mathbf{U}}(t, t_0) \right] = 0$$

□

## 10.4 (Commutators)

Calculation of the commutators of occupation number operator  $\hat{\mathbf{n}}_{\alpha} = \hat{\mathbf{a}}_{\alpha}^{\dagger} \hat{\mathbf{a}}_{\alpha}$  with the creator  $\hat{\mathbf{a}}_{\beta}^{\dagger}$  and annihilator  $\hat{\mathbf{a}}_{\beta}$ :

$$\left[ \hat{\mathbf{n}}_{\alpha}, \hat{\mathbf{a}}_{\beta}^{\dagger} \right]_{-} \quad \text{and} \quad \left[ \hat{\mathbf{n}}_{\alpha}, \hat{\mathbf{a}}_{\beta} \right]_{-}$$

we start with:

$$\left[ \hat{\mathbf{n}}_{\alpha}, \hat{\mathbf{a}}_{\beta}^{\dagger} \right]_{-} = \left[ \hat{\mathbf{a}}_{\alpha}^{\dagger} \hat{\mathbf{a}}_{\alpha}, \hat{\mathbf{a}}_{\beta}^{\dagger} \right]_{-} = \hat{\mathbf{a}}_{\alpha}^{\dagger} \hat{\mathbf{a}}_{\alpha} \hat{\mathbf{a}}_{\beta}^{\dagger} - \hat{\mathbf{a}}_{\beta}^{\dagger} \hat{\mathbf{a}}_{\alpha}^{\dagger} \hat{\mathbf{a}}_{\alpha}$$

using:



$$[AB, C] = ABC - CAB = ABC - \underbrace{ACB + ACB}_{=0} - CAB = A[B, C] + [A, C]B$$

we get:

$$[\hat{n}_\alpha, \hat{a}_\beta^+]_- = \hat{a}_\alpha^\dagger [\hat{a}_\alpha, \hat{a}_\beta^+]_- + [\hat{a}_\alpha^\dagger, \hat{a}_\beta^+]_- \hat{a}_\alpha$$

with  $[\hat{a}_\alpha, \hat{a}_\beta^+]_- = \delta_{\alpha\beta}$  and  $[\hat{a}_\alpha^\dagger, \hat{a}_\beta^+]_- = 0$  from the lecture we get for Bosons:

$$\begin{aligned} [\hat{n}_\alpha, \hat{a}_\beta^+]_- &= \hat{a}_\alpha^\dagger \delta_{\alpha\beta} + 0 \\ &= \hat{a}_\alpha^\dagger \delta_{\alpha\beta} \end{aligned}$$

for Fermions we got  $[\hat{a}_\alpha, \hat{a}_\beta^+]_+ = \hat{a}_\alpha \hat{a}_\beta^+ + \hat{a}_\beta^+ \hat{a}_\alpha = \delta_{\alpha\beta} \Leftrightarrow [\hat{a}_\alpha, \hat{a}_\beta^+]_- = \delta_{\alpha\beta} - 2\hat{a}_\beta^+ \hat{a}_\alpha$  and  $[\hat{a}_\alpha^\dagger, \hat{a}_\beta^+]_+ = \hat{a}_\alpha^\dagger \hat{a}_\beta^+ + \hat{a}_\beta^+ \hat{a}_\alpha^\dagger = 0 \Leftrightarrow [\hat{a}_\alpha^\dagger, \hat{a}_\beta^+]_- = -2\hat{a}_\beta^+ \hat{a}_\alpha^\dagger$ , therefore:

$$\begin{aligned} [\hat{n}_\alpha, \hat{a}_\beta^+]_- &= \hat{a}_\alpha^\dagger (\delta_{\alpha\beta} - 2\hat{a}_\beta^+ \hat{a}_\alpha) - 2\hat{a}_\beta^+ \hat{a}_\alpha^\dagger \hat{a}_\alpha \\ &= \hat{a}_\alpha^\dagger \delta_{\alpha\beta} - 2 [\hat{a}_\alpha^\dagger, \hat{a}_\beta^+]_+ \hat{a}_\alpha \\ &= \hat{a}_\alpha^\dagger \delta_{\alpha\beta} \end{aligned}$$

This means the relation is equal for Bosons and Fermions.

Now for the commutator with the annihilator:

$$\begin{aligned} [\hat{n}_\alpha, \hat{a}_\beta]_- &= [\hat{a}_\alpha^\dagger \hat{a}_\alpha, \hat{a}_\beta]_- \\ &= \hat{a}_\alpha^\dagger [\hat{a}_\alpha, \hat{a}_\beta]_- + [\hat{a}_\alpha^\dagger, \hat{a}_\beta]_- \hat{a}_\alpha \end{aligned}$$

with  $[\hat{a}_\alpha, \hat{a}_\beta]_- = 0$  and  $[\hat{a}_\alpha^\dagger, \hat{a}_\beta]_- = -[\hat{a}_\beta, \hat{a}_\alpha^\dagger]_- = -\delta_{\alpha\beta}$ , for Bosons:

$$\begin{aligned} [\hat{n}_\alpha, \hat{a}_\beta]_- &= 0 - \delta_{\alpha\beta} \hat{a}_\alpha \\ &= -\hat{a}_\alpha \delta_{\alpha\beta} \end{aligned}$$

and for Fermions ( $[\hat{a}_\alpha^\dagger, \hat{a}_\beta]_+ = \hat{a}_\alpha^\dagger \hat{a}_\beta + \hat{a}_\beta \hat{a}_\alpha^\dagger = [\hat{a}_\beta, \hat{a}_\alpha^\dagger]_+ = \delta_{\alpha\beta} \Leftrightarrow [\hat{a}_\alpha^\dagger, \hat{a}_\beta]_- = \delta_{\alpha\beta} - 2\hat{a}_\beta \hat{a}_\alpha^\dagger$  and  $[\hat{a}_\alpha, \hat{a}_\beta]_+ = \hat{a}_\alpha \hat{a}_\beta + \hat{a}_\beta \hat{a}_\alpha = 0 \Leftrightarrow [\hat{a}_\alpha, \hat{a}_\beta]_- = -2\hat{a}_\beta \hat{a}_\alpha$ ):

$$\begin{aligned} [\hat{n}_\alpha, \hat{a}_\beta]_- &= -2\hat{a}_\alpha^\dagger \hat{a}_\beta \hat{a}_\alpha + (\delta_{\alpha\beta} - 2\hat{a}_\beta \hat{a}_\alpha^\dagger) \hat{a}_\alpha \\ &= \hat{a}_\alpha \delta_{\alpha\beta} - 2 [\hat{a}_\alpha^\dagger, \hat{a}_\beta]_+ \hat{a}_\alpha \\ &= -\hat{a}_\alpha \delta_{\alpha\beta} \end{aligned}$$

Again we got the same result for Bosons and Fermions.