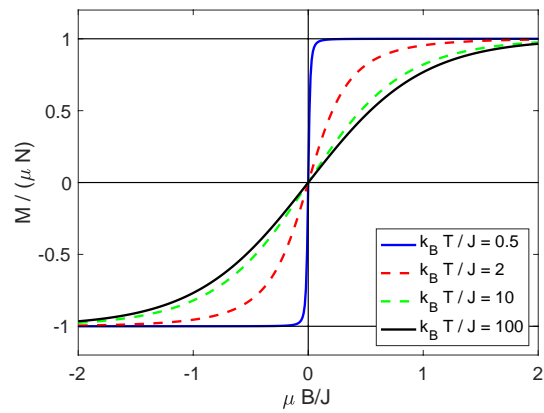
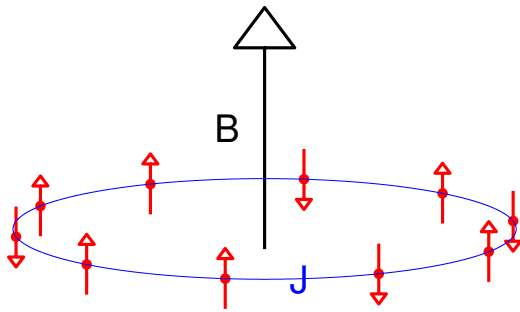


Advanced Statistical Physics (preliminary draft)

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(Stand 6.2.2017)



$$M(T, N, B) = N\mu \frac{\sinh(\mu\beta B)}{\sqrt{\sinh^2(\mu\beta B) + e^{-4J\beta}}}$$

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Chapter 1

Ising Model

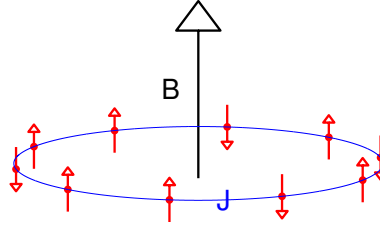


Figure 1.1: *Arrangement of Ising-spins in a 1d chain with pbc.*

We will now examine collective magnetism. The simplest model for this purpose is the Ising model, which is described by the following Hamilton function

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - B \hat{M} \quad (1.1)$$

$$\text{with } \hat{M} = \mu \sum_i S_i, \quad \left(\mu := -\frac{\mu_B g_e}{2} \right) \quad (1.2)$$

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - \mu B \sum_i S_i, \quad (1.3)$$

where the spins S_i can only take the values $S_i = \pm 1$. μ_B is the Bohr magneton and g_e the electronic Landé factor. J is the exchange coupling and the sum over sites is restricted to nearest neighbour sites, **such that each neighbouring pairings only counted once!** B stands for the magnetic flux density. The Ising model is also used to describe binary alloys. However, the parameters then have a different meaning. The Ising model can be solved exactly in 1d and 2d and in 2d it even has a phase transition. We consider periodic boundary

conditions ¹

1.1 Exact solution in 1D

The Hamilton function of the Ising model in 1D reads

$$H = -J \sum_{i=1}^N S_i S_{i+1} - \mu B \frac{1}{2} \sum_i (S_i + S_{i+1})$$

(pbc): $S_{i+N} = S_i$.

Canonical partition function

The evaluation is particularly simply in the canonical ensemble:

$$\begin{aligned} Z(T, N, B) &= \sum_{\{S_i\}=\pm 1} e^{\beta J \sum_i S_i S_{i+1} + \frac{\mu \beta B}{2} \sum_i (S_i + S_{i+1})} \\ &= \sum_{\{S_i\}=\pm 1} \prod_{i=1}^N e^{j S_i S_{i+1} + \frac{b}{2} (S_i + S_{i+1})} . \end{aligned}$$

We introduced the abbreviations $j = \beta J$ and $b = \mu B \beta$. We also define the **Transfermatrix**

$$\mathcal{T}_{s,s'} := e^{j s s' + \frac{b}{2} (s+s')} \quad (1.4a)$$

which has the matrix elements

$$\mathcal{T}_{s,s'} = \begin{array}{c|cc} & +1 & -1 \\ \hline +1 & e^{j+b} & e^{-j} \\ -1 & e^{-j} & e^{j-b} \end{array} \quad (1.4b)$$

then:

$$Z(T, N, B) = \sum_{\{S_i\}=\pm 1} \prod_{i=1}^N \mathcal{T}_{S_i, S_{i+1}} . \quad (1.4c)$$

We first consider the case $N = 2$, where the partition function reads

$$Z(T, N = 2, B) = \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \mathcal{T}_{s_1, s_2} \mathcal{T}_{s_2, s_1} = \sum_{s_1} (\mathcal{T}^2)_{s_1, s_1} = \text{tr} \{ \mathcal{T}^2 \}$$

The generalization to $N > 2$ leads obviously to

$$Z(T, N, B) = \text{tr} \{ \mathcal{T}^N \} .$$

¹In most cases, boundary conditions are irrelevant in the thermodynamic limits.

The transfer matrix is real-symmetric and can be expressed in the spectral representation as follows

$$\mathcal{T} = UDU^\dagger ,$$

here U is the unitary matrix of eigenvectors and D the diagonal matrix of eigenvalues (d_1, d_2) . Hence we have

$$\begin{aligned} Z(T, N, B) &= \text{tr} \{ \mathcal{T}^N \} = \text{tr} \{ (UDU^\dagger)^N \} = \text{tr} \{ UD^N U^\dagger \} = \text{tr} \{ D^N \} \\ &= d_1^N + d_2^N . \end{aligned}$$

The eigenvalues of the transfer matrix are

$$\begin{aligned} d_{1/2} &= \frac{e^{j+b} + e^{j-b}}{2} \pm \sqrt{\left(\frac{e^{j+b} - e^{j-b}}{2} \right)^2 + e^{-2j}} \\ &= e^j \left(\cosh(b) \pm \sqrt{\sinh^2(b) + e^{-4j}} \right) \end{aligned}$$

We can use $d_1 > d_2$ in the calculation of the partition function in thermodynamic limits

$$Z(T, N, B) = d_1^N \left[1 + \left(\frac{d_2}{d_1} \right)^N \right] .$$

Free energy

The free energy reads

$$\begin{aligned} F(T, N, B) &= -k_B T \ln [Z(T, B)] = -k_B T N \ln(d_1) - k_B T \ln \left[1 + \underbrace{\left(\frac{d_2}{d_1} \right)^N}_{\rightarrow 0} \right] \\ &= -Nk_B T \ln(d_1) . \end{aligned}$$

Magnetization

The mean magnetization is

$$M = \mu \left\langle \sum_i S_i \right\rangle .$$

The comparison with the partition function immediately shows

$$\begin{aligned}
M &= \frac{1}{\beta} \left(\frac{\partial \ln(Z)}{\partial B} \right) \Big|_{T,N} = - \left(\frac{\partial F}{\partial B} \right) \Big|_{T,N} \\
&= -\mu\beta \left(\frac{\partial F}{\partial b} \right) \Big|_{T,N} \\
&= -\mu\beta(-k_B T N) \left(\frac{\partial \ln(d_1)}{\partial b} \right) \Big|_{T,N} \\
&= N\mu \frac{\frac{\partial d_1}{\partial b}}{d_1} = N\mu \frac{\sinh(b) + \frac{\sinh(b) \cosh(b)}{\sqrt{\sinh^2(b) + e^{-4j}}}}{\cosh(b) + \sqrt{\sinh^2(b) + e^{-4j}}} \\
&= N\mu \sinh(b) \frac{1 + \frac{\cosh(b)}{\sqrt{\sinh^2(b) + e^{-4j}}}}{\cosh(b) + \sqrt{\sinh^2(b) + e^{-4j}}} \\
&= N\mu \frac{\sinh(b)}{\sqrt{\sinh^2(b) + e^{-4j}}} \frac{\sqrt{\sinh^2(b) + e^{-4j}} + \cosh(b)}{\cosh(b) + \sqrt{\sinh^2(b) + e^{-4j}}} .
\end{aligned}$$

MAGNETIZATION OF THE 1D ISING MODEL

$M(T, N, B) = N\mu \frac{\sinh(\mu\beta B)}{\sqrt{\sinh^2(\mu\beta B) + e^{-4J\beta}}} .$

1.1.1 Paramagnet

Without interaction of the magnetic moments ($J = 0$) we obtain

$$M(T, N, B) = N\mu \frac{\sinh(\mu\beta B)}{\sqrt{\sinh^2(\mu\beta B) + 1}} = N\mu \tanh(\mu\beta B) ,$$

the well-known result for paramagnetism.

1.1.2 Limits

It depends on the order of the limits. If we first set $B = 0$, we obtain for any finite temperature

$$M(T, N, B = 0) = 0$$

a vanishing magnetization. In the opposite order, i.e. keeping $B > 0$ finite and let T go to zero, i.e. $\beta \rightarrow \infty$ we obtain

$$M(T, B \neq 0) = N\mu \frac{\sinh(\mu\beta B)}{\sqrt{\underbrace{\sinh^2(\mu\beta B)}_{\gg 1} + \underbrace{e^{-4J\beta}}_{\ll 1}}}$$

$$\xrightarrow{T \rightarrow 0} N\mu \operatorname{sign}(B) .$$

In this limiting case we get perfect alignment of all spins, even if we now let B go to zero.

The Ising model in one dimension has a "phase transition" at $T = 0$.

1.1.3 Magnetization

We use the exchange coupling J as energy unit. Then two independent parameters remain, $k_B T$ and $\tilde{B} := \mu B$. We plot magnetization as a function of \tilde{B}

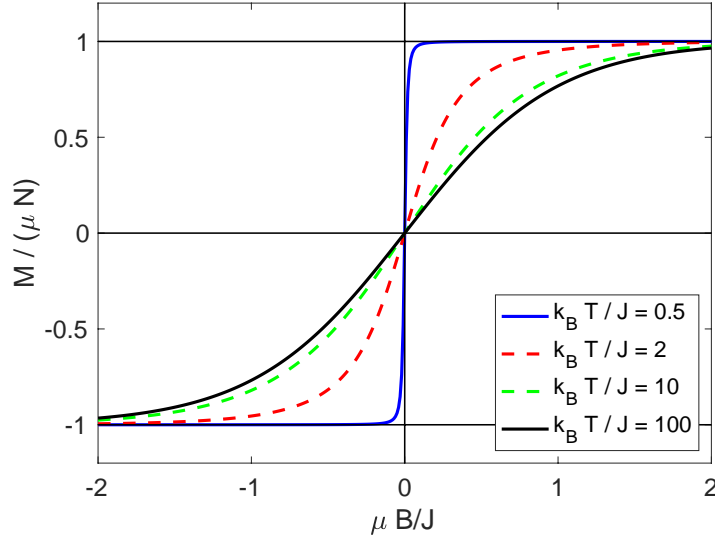


Figure 1.2: Magnetization curve of the 1d Ising model.

We can see from the comparison with the result for the paramagnet that the amount of magnetization increases everywhere due to the influence of the interaction. For low temperatures, the magnetization abruptly enters the fully polarized state.

1.2 Mean field approximation for any dimension

(See *Ising Model for Magnetism (Springer)*)

We will study the concept of the mean-field approximation in terms of the Ising model. We start out from the Ising model expressed as

$$H = -J \sum_{\langle ij \rangle} S_i S_j - B \cdot \hat{M}$$

We recall that the Ising model describes spin-1/2 objects. The total magnetisation \mathbf{M} is related to the spins via

$$\hat{M} = \mu \sum_i S_i .$$

Now the Ising model takes only the component along the quantization axis into account and S_i^z takes the values $\frac{\hbar}{2}\sigma_i$, with $\sigma_i \in \{-1, +1\}$. As before, we introduce the variable

$$h = \mu B .$$

and obtain

$$H = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i$$

The mean field approximation is defined for any two dynamical variables A and B by

$$AB \approx \langle A \rangle B + A \langle B \rangle - \langle A \rangle \langle B \rangle .$$

In our case, assuming translational invariance, we have

$$S_i S_j \approx \langle S \rangle S_j + S_i \langle S \rangle - \langle S \rangle^2 .$$

This leads to the mean-field Hamilton function

$$\begin{aligned} H_{\text{MFA}} &= -J \sum_{\langle ij \rangle} \langle S \rangle S_i - J \sum_{\langle ij \rangle} \langle S \rangle S_j + J \sum_{\langle ij \rangle} \langle S \rangle^2 - h \sum_i S_i \\ &= -2J \langle S \rangle \sum_{\langle ij \rangle} S_i + J \sum_{\langle ij \rangle} \langle S \rangle^2 - h \sum_i S_i \end{aligned}$$

Since we have used the convention that the sum over nearest neighbours avoids double counting, each site i has $z/2$ nearest neighbours, where for sc.lattices $z = 2d$ is defined as the total number of nearest neighbours. Hence:

$$H_{\text{MFA}} = -Jz \sum_i \langle S \rangle S_i + JNz \langle S \rangle^2 - h \sum_i S_i .$$

This can also be written as

$$H_{\text{MFA}} = -h' \sum_i S_i + \frac{JNz}{2} \langle S \rangle^2 \quad (1.5)$$

$$\text{with} \quad h' = h + Jz \langle S \rangle . \quad (1.6)$$

The canonical partition function is then given by

$$Z(T, N, B) = e^{-\frac{\beta N J z}{2} \langle S \rangle^2} \sum_{\{S_i\}} e^{\beta h' \sum_i S_i} , \quad (1.7)$$

The partition function can easily be computed

$$\begin{aligned} Z(T, N, B) &= e^{-\frac{\beta N J z}{2} \langle S \rangle^2} \prod_i \sum_{S_i = \pm 1} e^{h' S_i} \\ &= \left(e^{-\frac{\beta J z}{2} \langle S \rangle^2} 2 \cosh(\beta h') \right)^N \end{aligned} \quad (1.8)$$

$$\ln(Z(T, N, B)) = N \left(-\frac{\beta J z}{2} \langle S \rangle^2 + \ln(2) + \ln(\cosh(\beta h')) \right) \quad (1.9)$$

1.2.1 Magnetization

Next we compute the mean magnetization

$$\frac{M}{\mu} = \frac{\langle \hat{M} \rangle}{\mu} = \frac{1}{Z} \sum_{\{S_i\}} \left\{ \hat{M} e^{-\frac{\beta N J z}{2} \langle S \rangle^2} e^{\beta h' \hat{M}} \right\} = \frac{k_B T}{Z} \frac{\partial}{\partial h'} Z .$$

$$\frac{M}{\mu} = k_B T \frac{\partial \ln(Z)}{\partial h'} = N \tanh(\beta h') . \quad (1.10)$$

We introduce the magnetization per site

$$m = \frac{M}{\mu N} = \frac{1}{N} \langle \sum_i S_i \rangle = \langle S \rangle . \quad (1.11)$$

and obtain the equation of state

<p>MAGNETIZATION (of the Ising model)</p> <hr style="border: 0.5px solid black;"/> $m = \tanh \left(\beta (J z m + h) \right) . \quad (1.12)$
--

We are particularly interested in the spontaneous magnetization, i.e. the magnetization for $B \rightarrow 0$. So we seek the solution of

$$m = \tanh(\beta J z m) . \quad (1.13)$$

We introduce an auxiliary temperature T^* , defined by

$$k_B T^* = J z . \quad (1.14)$$

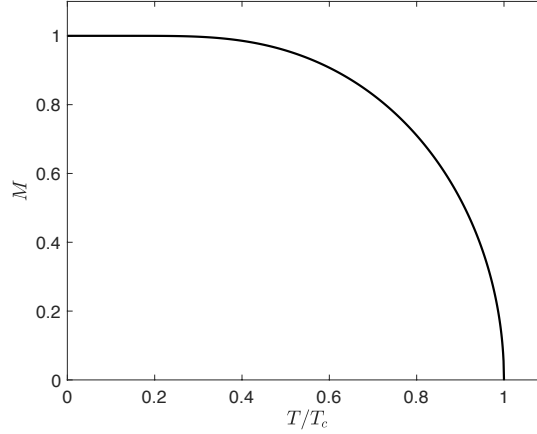


Figure 1.3: *Mean-field result for the Magnetization for arbitrary spatial dimension d*

The condition for the spontaneous magnetization can therefore be expressed in a form, independent of the dimension

$$m = \tanh\left(\frac{T^*}{T}m\right) \quad (1.15)$$

or rather with $x = \frac{T^*}{T}m$

$$x = \frac{T^*}{T} \tanh(x) . \quad (1.16)$$

The function $\tanh(x)$ starts at $x = 0$ with the value 0 and slope 1, then it increases monotonically with decreasing slope and approaches 1 for $x \rightarrow \infty$. equation (1.16) has always the trivial solution $M = 0$. For the non-trivial solution, we need $\frac{T^*}{T} > 1$, or rather $T < T^*$. According to the behaviour of $\tanh(x)$, for $\frac{T^*}{T} > 1$ there is precisely one non-trivial solution. So we see that T^* is indeed the critical/ Curie temperature, i.e

$$k_B T_C = Jz . \quad (1.17)$$

In 2D, we have $(\beta_c J) = .25$, as compared to the exact value $\beta_c J = 0.4407$. This not so bad, however, for 1D the mean-field result predicts a phase-transition at $(\beta_c J) = .5$, while the exact result is ∞ .

In figure 1.3, the magnetization, obtained from equation (1.13) [\[previous page\]](#) , is depicted as function of T . Interestingly, the curve is independent of the spatial dimension. The later only enters in the value of T_c

Critical exponent

For temperatures T slightly below T_c , the magnetization is very small and we can use the Taylor expansion with $\tau = T/T_C$

$$\begin{aligned} m &= \tanh\left(\frac{m}{\tau}\right) = \left(\frac{m}{\tau} - \frac{(m/\tau)^3}{3}\right) = \frac{m}{\tau} \left(1 - \frac{(m/\tau)^2}{3}\right) \\ \tau &= 1 - \frac{(m/\tau)^2}{3} \\ \left(\frac{m}{\tau}\right)^2 &= 3\left(1 - \tau\right). \end{aligned}$$

Up to this order we have for $T < T_C$

$$m = 3\tau\sqrt{1-\tau} \propto \varepsilon^{\frac{1}{2}} \quad (1.18)$$

$$\varepsilon := \frac{T_C - T}{T_C} \quad (1.19)$$

The critical exponent is therefore $\beta = 1/2$.

1.2.2 Magnetic susceptibility

Starting from the definition of the susceptibility via

$$\chi = \left. \frac{\partial M}{\partial B} \right|_{T, h=0}$$

we obtain with $M = mN\mu$ and $B = h/\mu$ the relation

$$\chi = \mu^2 N \left. \frac{\partial m}{\partial h} \right|_{T, h=0}$$

We start out from

$$m = \tanh\left(\beta h + \frac{T_C}{T} m\right)$$

The derivative w.r.t. h is

$$\begin{aligned} \xi &= \left. \frac{\partial m}{\partial h} \right|_{T, h=0} = \left. \frac{\beta + \frac{T_C}{T} \xi}{\cosh^2\left(\beta h + \frac{T_C}{T} m\right)} \right|_{h=0} = \frac{\beta + \frac{T_C}{T} \xi}{\cosh^2\left(\frac{T_C}{T} m\right)} \\ \xi \cosh^2\left(\frac{T_C}{T} m\right) &= \beta + \frac{T_C}{T} \xi \\ \xi \left(\cosh^2\left(\frac{T_C}{T} m\right) - \frac{T_C}{T} \right) &= \beta. \end{aligned}$$

Close to T_C the magnetisation is very small and we can Taylor expand the magnetisation resulting in

$$\begin{aligned}\xi &= \frac{\beta}{\cosh^2\left(\frac{T_C}{T}m\right) - \frac{T_C}{T}} \\ &= \frac{\beta}{1 - \frac{T_C}{T} + \left(\frac{T_C}{T}m\right)^2} \\ &= \frac{1}{k_B} \frac{1}{T - T_C + T_C \frac{T_C}{T} m^2} .\end{aligned}$$

We can replace T by T_C in the last term in the denominator, as it already contains $O(m^2)$

$$\xi = \frac{1}{k_B} \frac{1}{T - T_C + T_C m^2} .$$

For $T \searrow T_C$ the magnetisation is zero and we have

$$\xi = \frac{1}{k_B T_C} (\varepsilon)^{-1}$$

with $\varepsilon = (T - T_C)/T_C$.

For $T \nearrow T_C$ we use equation (1.18) [\[previous page\]](#) for m and obtain

$$m^2 = 3\tau^2(1 - \tau) = \frac{3}{T_C}(T_C - T) + \mathcal{O}(\Delta T/T_C)^2$$

and have

$$\xi = \frac{1}{k_B} \frac{1}{T - T_C + 3(T_C - T)} = \frac{1}{2k_B T_C} |\varepsilon|^{-1}$$

According to the definition of the critical exponent of the susceptibility

$$\chi \simeq A_{\pm} |\varepsilon|^{-\gamma_{\pm}}$$

we have $A_+ = 2A_-$ and $\gamma_+ = \gamma_- = 1$.

1.2.3 Free energy

Next we compute the free energy based equation (1.9) [\[p. 11\]](#)

$$\begin{aligned}f &:= \frac{F}{k_B N} = -\frac{k_B T}{k_B N} \ln(Z) \\ &= -T \left(-\frac{\beta J z}{2} \langle S \rangle^2 + \ln(2) + \ln(\cosh(\beta h')) \right) \\ &= \frac{J z}{2 k_B} m^2 - T \ln(2) - T \ln\left(\cosh\left(\beta h + \frac{J z}{k_B T} m\right)\right) .\end{aligned}$$

We have seen before that $k_B T_C = Jz$ so we can express the free energy as

$$\frac{F}{Nk_B} = \frac{1}{2}T_c m^2 - T \ln(2) - T \cosh(\beta h + \frac{T_c}{T}m) .$$

Along with

$$\cosh(x) = (1 - \tanh^2(x))^{-1/2}$$

and the self consistency equation (1.15) [p. 12]

$$m = \tanh\left(\beta h + \frac{T_c}{T}m\right) \quad (1.20)$$

we can express the free energy as

$$\frac{F}{Nk_B} = \frac{T_c m^2}{2} - T \ln(2) + \frac{T}{2} \ln(1 - m^2) \quad (1.21)$$

Next we compute the Helmholtz free energy, by the following Legendre transform, i.e. by introducing M as natural variable instead of h :

$$A(T, M) = F(T, h) + Mh . \quad (1.22)$$

Then the total differential reads

$$\begin{aligned} dA &= dF(T, h) + h dM + M dh \\ &= -S dT - M dh + h dM + M dh \\ &= -S dT + h dM . \end{aligned}$$

Hence

$$\left. \frac{\partial A}{\partial M} \right|_T = h \quad (1.23)$$

$$\left. \frac{\partial A}{\partial T} \right|_M = -S . \quad (1.24)$$

If we want to have spontaneous magnetisation, i.e. a finite magnetisation M without external field, then according to equation (1.23) we are looking for a finite value of the magnetization M for which

$$\left. \frac{\partial A(M, T)}{\partial M} \right|_T = 0 . \quad (1.25)$$

Before we can exploit this equation, we need to express h in terms of M (or rather m). To this end we invert

$$m = \tanh\left(\beta h + \frac{T_c}{T}m\right)$$

leading to

$$\beta h + \frac{T_C}{T} m = \tanh^{-1}(m) .$$

Along with

$$\tanh^{-1}(b) = \frac{1}{2} \ln \left(\frac{1+b}{1-b} \right)$$

we obtain

$$\begin{aligned} \beta h + \frac{T_c}{T} m &= \frac{1}{2} \ln \left(\frac{1+m}{1-m} \right) \\ h &= \frac{k_B T}{2} \ln \left(\frac{1+m}{1-m} \right) - k_B T_c m \end{aligned}$$

Then we obtain for the Helmholtz free energy of equation (1.21) [\[previous page\]](#)

$$\begin{aligned} \frac{A}{Nk_B} &= \frac{T_C m^2}{2} - T \ln(2) + \frac{T}{2} \ln(1-m^2) + \frac{mh}{k_B} \\ &= \frac{1}{2} T_c m^2 - T \ln(2) + \frac{T}{2} \ln(1-m^2) + \frac{m}{k_B} \left(\frac{k_B T}{2} \ln \left(\frac{1+m}{1-m} \right) - k_B T_c m \right) \\ &= \frac{1}{2} T_c m^2 - T \ln(2) + \frac{T}{2} \ln(1-m^2) + \frac{mT}{2} \ln \left(\frac{1+m}{1-m} \right) - T_c m^2 . \end{aligned}$$

or rather

$$\begin{aligned} \frac{A}{Nk_B T_c} &= \frac{A}{NJz} = -\frac{1}{2} m^2 - \tau \ln(2) + \frac{\tau}{2} \left[\ln((1-m)(1+m)) + m \ln \left(\frac{1+m}{1-m} \right) \right] \\ &= -\frac{1}{2} m^2 - \tau \ln(2) + \frac{\tau}{2} \left((1+m) \ln(1+m) + (1-m) \ln(1-m) \right) , \end{aligned} \tag{1.26}$$

with $\tau = T/T_c$. According to equation (1.25) [\[previous page\]](#) the magnetization is given by the points where the slope as function of τ vanishes (see figure 1.4).

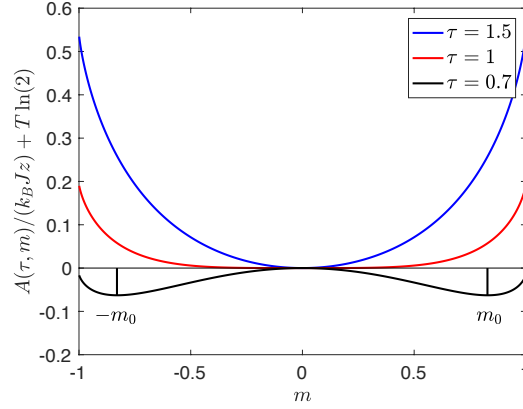


Figure 1.4: *Helmholtz free energy for the Ising model in mean-field approximation versus order parameter without external field.*

1.2.4 Entropy

According to equation (1.23) [p. 15] along with equation (1.26) [previous page] the entropy is

$$-\frac{S}{Nk_B T_C} = \frac{\partial}{\partial \tau} \left(-\frac{1}{2}m^2 - \tau \ln(2) + \frac{\tau}{2} \left((1+m) \ln(1+m) + (1-m) \ln(1-m) \right) \right) \bigg|_m \frac{d\tau}{dT}.$$

Hence

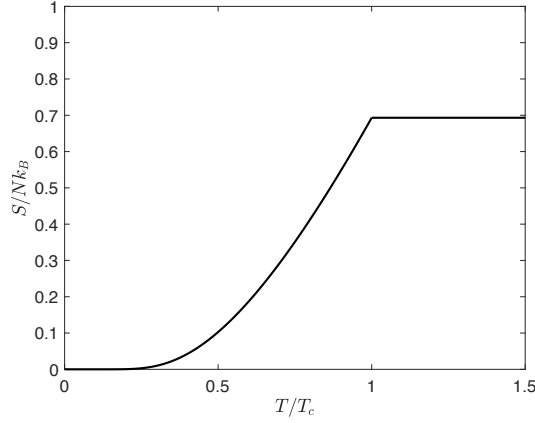
<p>ENTROPY OF THE ISING MODEL (in MFA for zero field)</p> <hr/> $\frac{S}{Nk_B} = \ln(2) - \frac{1}{2} \left((1+m) \ln(1+m) + (1-m) \ln(1-m) \right). \quad (1.27)$
--

It has the correct limiting behaviour: For $T \rightarrow 0$, i.e. $m \rightarrow 1$ we obtain

$$\frac{S}{Nk_B} = \ln(2) - \frac{1}{2} \left(2 \left(\ln(2) + 0 \right) \right) = 0,$$

and for $T \rightarrow \infty$, i.e. $m \rightarrow 0$ the entropy becomes

$$\frac{S}{Nk_B} = \ln(2) - \frac{1}{2} \left(\ln(1) + \ln(1) \right) = \ln(2).$$

Figure 1.5: *Entropy of the Ising model in MFA.*

Recall that

$$S = k_B \ln(\text{number of micro states}) .$$

For $T \rightarrow \infty$ all states can be reach with the same probability. Hence the number of micro states is 2^N and

$$S = Nk_B \ln(2) ,$$

kin agreement with the above result.

For the entire T dependence of S we have to insert the self-consistent solution for $m(T)$ in equation (1.15) [\[p. 12\]](#).

1.2.5 Internal energy

The internal energy is defined as the expectation value of the hamiltonian. Using the mean field expression of equation (1.5) [\[p. 10\]](#) we have

$$U = \langle H \rangle = -h' \sum_i \langle S_i \rangle + \frac{JNz}{2} m^2 = N \left(-h' m + \frac{Jz}{2} m^2 \right)$$

with $h' = Jzm + h$ we obtain:

$$\begin{aligned} \frac{U}{N} \frac{1}{NJ} &= -\frac{hm}{J} - zm^2 + \frac{z}{2} m^2 \\ &= -\frac{z}{2} m^2 - \frac{hm}{J} . \end{aligned}$$

For zero external field it simplifies to (we also use $z = 2d$)

INTERNAL ENERGY OF THE ISING MODEL
(in MFA for zero field)

$$\frac{U}{NJ} = -d m^2 . \quad (1.28)$$

1.2.6 Specific heat

For the specific heat we need

$$\begin{aligned} C_{h=0} &= \left. \frac{\partial U}{\partial T} \right|_{h=0} = -dNJ \frac{d m^2}{dT} \\ \frac{C_{h=0}}{NJ} &= -d \frac{d}{dT} m^2 . \end{aligned}$$

Above T_C the magnetization is zero and hence $C = 0$. Slightly below T_C we can replace m by equation (1.18) [p. 13], which gives

$$\begin{aligned} \frac{C_{h=0}}{NJ} &= -d \frac{d}{dT} 3\tau^2 (1 - \tau) \\ &= -\frac{3d}{T_C^3} \frac{d}{dT} (T^2 T_C - T^3) \\ &= -\frac{3d}{T_C^3} T (2T_C - 3T) . \end{aligned}$$

Hence, approaching T_C from below we obtain

$$\begin{aligned} \frac{C(T_C)_{h=0}}{NJ} &= \frac{3d}{T_C} = \frac{3dk_B}{Jz} = \frac{3dk_B}{J2d} \\ \frac{C(T_C)_{h=0}}{N} &= \frac{3k_B}{2} . \end{aligned}$$

Therefore, in MFA, the specific heat has no power-law behaviour close at T_C , but rather a discontinuity from $\frac{3}{2}k_B$ below T_C to 0 above T_C . For the entire T -dependence below T_C we continue

$$\frac{C_{h=0}}{NJ} = -2d m \frac{dm}{dT} . \quad (1.29)$$

First we consider

$$\xi := \frac{dm}{dT} .$$

Exploiting equation (1.20) [p. 15] yields

$$\xi = \frac{d}{dT} \tanh(\beta h + \beta k_B T_C m) \Big|_{h=0} \quad (1.30)$$

$$\xi = \frac{(h + k_B T_C m) \frac{d\beta}{dT} + \beta k_B T_C \xi}{\cosh^2(\beta(h + k_B T_C m))} \Big|_{h=0} \quad (1.31)$$

$$= \frac{-\frac{T_c}{T^2} m + \frac{T_C}{T} \xi}{\cosh^2\left(\frac{T_C}{T} m\right)} . \quad (1.32)$$

Then

$$\begin{aligned} \xi \cosh^2\left(\frac{T_C}{T} m\right) &= -\frac{T_c}{T^2} m + \frac{T_C}{T} \xi \\ \xi \left(\cosh^2\left(\frac{T_C}{T} m\right) - \frac{T_C}{T} \right) &= -\frac{T_c}{T^2} m \\ \xi &= -\frac{1}{T_C} \frac{\frac{m}{\tau}}{\tau \cosh^2\left(\frac{m}{\tau}\right) - 1} \end{aligned}$$

Finally, we have

$$\begin{aligned} \frac{C_{h=0}}{NJ} &= -z m \xi \\ &= \frac{z}{T_C \tau} \frac{\frac{m^2}{\tau}}{\cosh^2\left(\frac{m}{\tau}\right) - 1} \\ &= \frac{z}{zJ/k_B \tau} \frac{\frac{m^2}{\tau}}{\cosh^2\left(\frac{m}{\tau}\right) - 1} . \end{aligned}$$

Finally, we have

$$\frac{C_{h=0}}{N} = k_B \frac{\left(\frac{m}{\tau}\right)^2}{\cosh^2\left(\frac{m}{\tau}\right) - 1/\tau} . \quad (1.33)$$

Together with the self consistent equation for $m(T)$:

$$m(T) = \tanh\left(\frac{T_C}{T} m(T)\right) ,$$

which have solved numerically before, we can plot the specific heat.

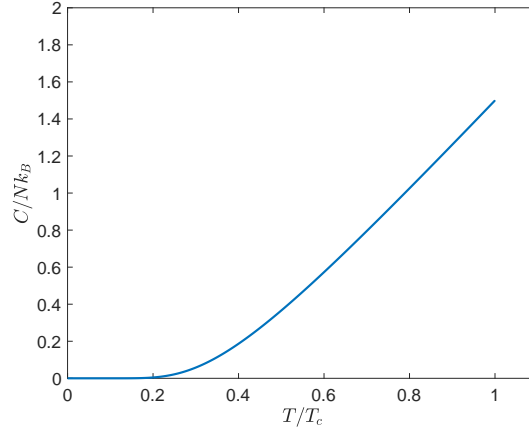


Figure 1.6: *Specific heat of the Ising model in MFA.*

We have seen 'statistical physics I'

$$C = \frac{1}{k_B T^2} \left\langle (\Delta H)^2 \right\rangle ,$$

i.e. C is large when there are pronounced energy fluctuations, which is the case in the vicinity of T_C . In MFA, above T_C there are no fluctuations because $H \propto m$ and therefore $U = 0$ above T_C . This is an artefact of MFA.

1.3 Exact solution of the 2d Ising model

1.3.1 Transfermatrix approach

We will first briefly explain how the Transfer matrix approach works in the 2d case. To this end we will represent the hamiltonian of the 2d Ising model ($L_x \times L_y$) by writing the two cartesian indices explicitly in the form S_{ij}

$$-\beta H = j \sum_{l=1}^{L_y} \sum_{i=1}^{L_x} S_{i,l} S_{i+1,l} + S_{i,l} S_{i,l+1} + h \sum_l \sum_i S_{il} .$$

Now we combine the spins of column l of S_{il} in a vector

$$\mathcal{S}^{(l)} = \begin{pmatrix} S_{1,l} \\ S_{2,l} \\ \vdots \\ S_{L_x,l} \end{pmatrix} , \text{ i.e. } (\mathcal{S}^{(l)})_i = S_{il}$$

Then the hamiltonian can be written as

$$-\beta H = \sum_l A(\mathcal{S}^{(l)}, \mathcal{S}^{(l+1)}) \quad (1.34)$$

with the definitions

$$A(\mathcal{S}^{(l)}, \mathcal{S}^{(k)}) = \frac{1}{2} \left(\tilde{A}(\mathcal{S}^{(l)}, \mathcal{S}^{(k)}) + \tilde{A}(\mathcal{S}^{(k)}, \mathcal{S}^{(l)}) \right) \quad (1.35)$$

$$\tilde{A}(\mathcal{S}^{(l)}, \mathcal{S}^{(k)}) = j \sum_i \left((\mathcal{S}^{(l)})_i (\mathcal{S}^{(l)})_{i+1} + (\mathcal{S}^{(l)})_i (\mathcal{S}^{(k)})_i \right) + h \left(\sum_i \mathcal{S}^{(l)}_i \right). \quad (1.36)$$

A is by construction a real symmetric matrix. Inserting indices yields

$$\begin{aligned} \sum_l \tilde{A}(\mathcal{S}^{(l)}, \mathcal{S}^{(l+1)}) &= j \sum_{l,i} (S_{i,l} S_{i+1,l} + S_{i,l} S_{i,l+1}) + h \sum_{i,l} S_{i,l} &= -\beta H \\ \sum_l \tilde{A}(\mathcal{S}^{(l+1)}, \mathcal{S}^{(l)}) &= j \sum_{l,i} (S_{i,l+1} S_{i+1,l+1} + S_{i,l+1} S_{i,l}) + h \sum_{i,l} S_{i,l+1} \\ (l+1 \rightarrow l' \text{ plus pbc} \Rightarrow) &= j \sum_{l',i} (S_{i,l'} S_{i+1,l'} + S_{i,l'} S_{i,l+1}) + h \sum_{i,l} S_{i,l'} &= -\beta H. \end{aligned}$$

Hence equation (1.34) is correct. Then

$$Z = \sum_{\{S_{ij}\}} e^{\sum_{l=1}^L A(\mathcal{S}^{(l)}, \mathcal{S}^{(l+1)})} = \prod_{l=1}^L \sum_{\mathcal{S}^{(l)}} e^{A(\mathcal{S}^{(l)}, \mathcal{S}^{(l+1)})}.$$

Now, we introduce the transfer matrix \mathcal{T} with matrix elements

$$\mathcal{T}_{\mathcal{S}^{(l)}, \mathcal{S}^{(l')}} = e^{A(\mathcal{S}^{(l)}, \mathcal{S}^{(l')})}$$

Then the partition function can be written as (remember that we use pbc)

$$\begin{aligned} Z &= \sum_{\mathcal{S}^{(1)}} \sum_{\mathcal{S}^{(2)}} \cdots \sum_{\mathcal{S}^{(L_y)}} \prod_l \mathcal{T}_{\mathcal{S}^{(l)}, \mathcal{S}^{(l+1)}} \\ &= \sum_{\mathcal{S}^{(1)}} \sum_{\mathcal{S}^{(2)}} \cdots \sum_{\mathcal{S}^{(L_y)}} \mathcal{T}_{\mathcal{S}^{(1)}, \mathcal{S}^{(2)}} \mathcal{T}_{\mathcal{S}^{(2)}, \mathcal{S}^{(3)}} \cdots \mathcal{T}_{\mathcal{S}^{(L_y-1)}, \mathcal{S}^{(L_y)}} \mathcal{T}_{\mathcal{S}^{(L_y)}, \mathcal{S}^{(1)}} \\ &= \text{tr} \{ \mathcal{T}^{L_y} \} \\ &= \lambda_{\max}^{L_y}. \end{aligned}$$

This is the straight-forward generalization of equation (1.4) [p. 5] and is to be understood as follows: The sum over $\mathcal{S}^{(l)}$ runs over the 2^{L_x} configurations,

which the vector $\mathcal{S}^{(l)}$ can assume. We introduce an index I that enumerates these configurations and instead of summing over $\mathcal{S}^{(l)}$, we could sum over the index I , that enumerates these configurations (the I -the configuration would be \mathcal{S}_I). Then we can define the transfer matrix alternatively by the matrix elements

$$\mathcal{T}_{I,I'} = e^{A(\mathcal{S}_I, \mathcal{S}_{I'})}$$

and then we would have

$$\begin{aligned} Z &= \sum_{I^{(1)}} \cdots \sum_{I^{(L_y)}} \mathcal{T}_{I^{(1)}, I^{(2)}} \mathcal{T}_{I^{(2)}, I^{(3)}} \cdots \mathcal{T}_{I^{(L_y-1)}, I^{(L_y)}} \mathcal{T}_{I^{(L_y)}, I^{(1)}} \\ &= \text{tr} \{ \mathcal{T}^{L_y} \} \\ &= \lambda_{\max}^N . \end{aligned}$$

As before, the dominant eigenvector (λ_{\max}) predominates in the thermodynamic limit ($L_y \rightarrow \infty$). The eigenvalue problem of the $(2^{L_x} \times 2^{L_x})$ -dimensional transfer matrix for the 2d case, is much more complicated than in the 1d case. It can be found in the book of K. Huang (*Kerson Huang, Statistical Mechanics, Wiley and Sons (1963)*).

1.3.2 Graphical approach

Here we will present instead the exact solution of the 2d Ising model based a graphical representation, however, without external field. The ideas go back to M. Lawrence Glasser, American Journal of Physics 38, 1033 (1970), and were didactically improved by W. Nöting: Quantum Theory of Magnetism (Springer Verlag).

Starting point is the partition function

$$Z = \sum_{\{S_i\}} \prod_{\langle ij \rangle} e^{j S_i S_j} . \quad (1.37)$$

Next we expand the exponential in a Taylor series

$$\begin{aligned} e^{j S_i S_j} &= \sum_{n=0}^{\infty} \frac{j^n}{n!} (S_i S_j)^n \\ &= \sum_{n=0}^{\infty} \frac{j^{2n}}{(2n)!} \underbrace{(S_i S_j)^{2n}}_{=1} + \sum_{n=0}^{\infty} \frac{j^{2n+1}}{(2n+1)!} \underbrace{(S_i S_j)^{2n+1}}_{=S_i S_j} \\ &= \cosh(j) (1 + \tanh(j) S_i S_j) \end{aligned}$$

Inserted in equation (1.37) results in

$$Z = \cosh^{2N}(j) \sum_{\{S_i\}} \prod_{\langle ij \rangle} (1 + t S_i S_j) ,$$

where $t = \tanh(j)$. The power $2N$ arises as there are $2N$ terms in the product in equation (1.37) [\[previous page\]](#). For each factor we have the choice to use the term 1 or $t S_i S_j$. In total there are 2^{Nz} such terms, for which we still have to sum over all spin configurations. Graphically, we represent the terms $t S_i S_j$ as lines on a square lattice connecting site i and j . Such a line can be considered as *edge of a graph* and the sites that are connected by edges are denoted as *vertices*. In graph theory the number of edges connected to a vertex is called *order of the vertex*. In the present context, it can only be an integer $n \in \{1, 2, 3, 4\}$. Each edge, that reaches site (vertex) i carries a factor S_i . Therefore, we obtain a term S_i^n , where n is the order of the vertex. $n \in \{0, 1, 2, 3, 4\}$. If the order is odd, the sum over S_i vanishes, otherwise it gives 2. Hence, only graphs where all vertices have an even order (either 2 or 4) are allowed. By now we have

$$Z = 2^N \cosh^{2N}(j) \sum_G t^{N_e(G)} ,$$

The sum runs over all possible graphs on a square lattice of given size, with periodic boundary conditions, with vertices of even order. $N_e(G)$ is the total number of edges of the graph. The elements of the individual graphs need not to be connected. In figure 1.7 two examples are given, one for an allowed and one for a forbidden graph. We can rewrite the sum over allowed graphs also in the form

$$Z = 2^N \cosh^{2N}(j) \left(1 + \sum_{n=4}^{\infty} g_n t^n \right) , \quad (1.38)$$

where n is the number of edges and g_n is the number of allowed graphs with n edges. We have already exploited that the smallest graph (besides the empty graph) has 4 edges. Since each vertex has even order, the allowed graphs contain closed paths, as can be seen in figure 1.7.

1.3.3 Making the graphs unique

The figure also contains a *node*, i.e. a vertex of order 4. Let's try to draw the graph with a pencil on a piece of squared paper. We start at an arbitrary vertex of order 2 and draw a line to one of the two connected vertices. If the next vertex also has order 2, it is obvious how to continue the drawing.

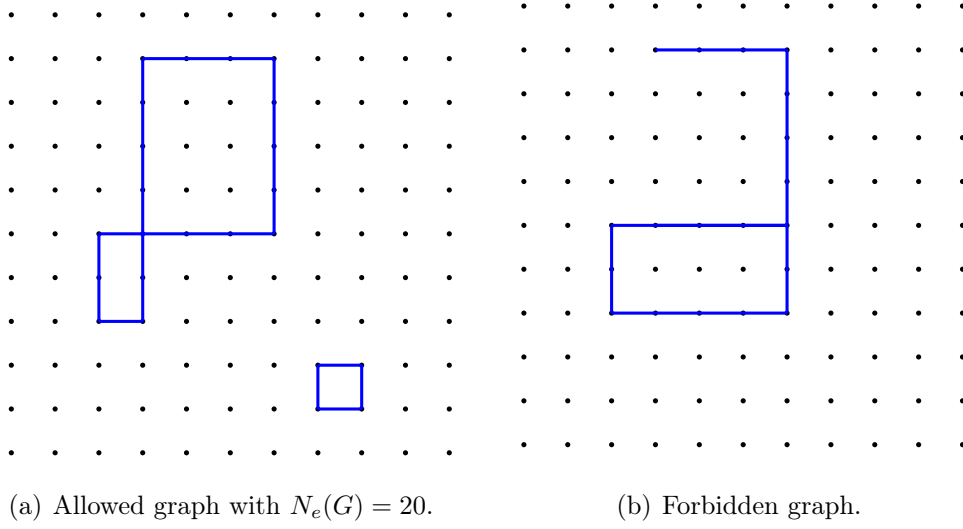


Figure 1.7: *Graphical representation of the partition function of the Ising model.*

When we reach a node, however, we have 3 options to continue: *turn left, go straight, turn right*. It will turn out to be advantageous, to replace the graph by objects that allow to draw them in a unique way. Therefore, we will introduce graphical objects, that make a node unique. To this end a node is split into the three graphical objects, shown in figure 1.8. This splitting

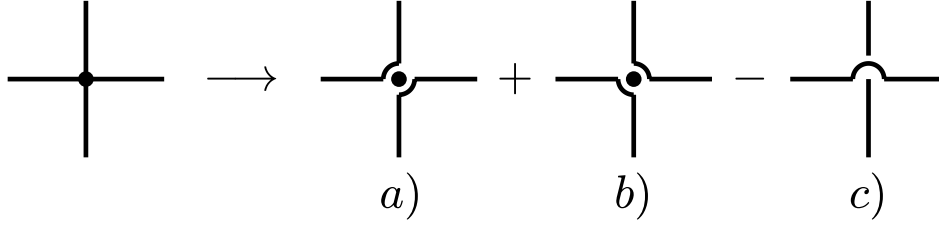


Figure 1.8: *Splitting of a node with corresponding weights.*

results in 3^{N_n} different new graphs, obtained from a graph with N_n nodes. This would increase g_n in a complicated way. To avoid this complication, each new graphical element obtains a weight factor ± 1 , as shown in figure 1.8. Now the three contributions of each node add up to 1 again and the total count does not change. The new graphs are denoted by \tilde{G} . They consist of one or more loops. As a remainder, a *loop* (with e.g. n edges) is a simply connected set of edges, i.e. an object that can be drawn by starting at an arbitrary vortex on the loop, following the edges, and returning at the

starting point after n steps. The shortest loop has 4 edges and the number of edges is always even. In the new graphs \tilde{G} , the number of edges has not changed, as compared to the original graph, but it has an extra weight factor

$$w(\tilde{G}) = (-1)^{N_c(\tilde{G})} ,$$

where $N_c(\tilde{G})$ stands for the number of **crossings** (decomposition c in figure 1.8) of a graph \tilde{G} of the new type. By now g_n is

$$g_n = \sum_{\tilde{G}}^{N_e(\tilde{G})=n} (-1)^{N_c(\tilde{G})} .$$

1.3.4 Decomposing graphs into loops

We are still not able to calculate the sum of all graphs analytically. To this end we need to transform the graphs further. Each graph \tilde{G} with n edges consists of one or more loops, which in total have n edges. If a particular graph \tilde{G} consists of l loops, we can divide the total weight between the loops. A loop L contributes a factor $(-1)^{N_c(L)}$, where $N_c(L)$ is the number of crossings in loop L . The total weight is the product of the weights of the loops of which the graph is formed. Clearly, there is a one-to-one correspondence between all graphs \tilde{G} with n edges and all sets of loops with a total number n of edges. We define

$$D_l = \begin{cases} \sum_L^{\text{loops with } l \text{ edges}} (-1)^{N_c(L)} & \text{if } l \text{ is even} \\ 0 & \text{otherwise} \end{cases} . \quad (1.39)$$

Hence for $n \geq 4$ we may think that we can decompose g_n into the contribution of the loop decomposition:

$$g_n = \sum_{\tilde{G}} \delta_{N_e(\tilde{G})=n} (-1)^{N_c(\tilde{G})} = \sum_{m=1}^{\infty} \frac{1}{m!} \sum_{l_1 \dots l_m=4} \delta_{\sum_{\nu=1}^m l_{\nu}=n} \prod_{\nu=1}^m D_{l_{\nu}} \quad (1.40)$$

Here m is the number of loops and l_{ν} stands for the number of edges of loop ν and $D_{l_{\nu}}$ is the corresponding weight obtained by summing over all realizations of a loop with l_{ν} edges. The factor $1/m!$ is required as the right hand side creates a particular set of m loops in $m!$ different permutations.

We can insert equation (1.40) in equation (1.38) [p. 24] and obtain

$$\begin{aligned}
\sum_{n=4}^{\infty} g_n t^n &= \sum_{m=1}^{\infty} \frac{1}{m!} \sum_{l_1 \dots l_m=4} \underbrace{\sum_{n=4}^{\infty} \delta_{\sum_{\nu=1}^m l_\nu=n}}_{=1} \prod_{\nu=1}^m D_{l_\nu} t^{l_\nu} \\
&= \sum_{m=1}^{\infty} \frac{1}{m!} \prod_{\nu=1}^m \left(\sum_{l=4}^{\infty} D_l t^l \right) \\
&= \sum_{m=1}^{\infty} \frac{1}{m!} \left(\sum_{l=4}^{\infty} D_l t^l \right)^m \\
&= \exp \left(\sum_{l=4}^{\infty} D_l t^l \right) - 1
\end{aligned}$$

Hence according to equation (1.38) [p. 24] we have

$$\ln(Z) = N \ln(2) + 2N \ln(\cosh(j)) + \sum_{m=1}^{\infty} D_m t^m. \quad (1.41)$$

The sum can start at $m = 1$ (instead of $m = 4$) since equation (1.39) [previous page] counts loops and the shortest loop has length 4 anyways. However, equation (1.40) [previous page] is not really correct. On the rhs the sum runs over all configurations of independently arranged loops. I.e. there will be configurations where edges occur more than once, like in figure 1.9. Such a configuration is not included in \tilde{G} . However, there is a very simple cure. We allow such configurations also in \tilde{G} , but in addition to double bonds, say, as in figure 1.9 a) or schematically depicted in figure 1.10 a) we also include configurations that occur if we cross the lines as shown in figure 1.10 b) and give them a weight -1 . The sum of these configurations adds up to zero. The same holds true, if there are threefold edges as in figure 1.9 b) or even m -fold edges. Generally, in the case of m -fold edges there are $m!$ possible connections (permutations) of the incoming and outgoing lines. The number of crossings is even/odd if the permutation is even/odd. As the number of even permutations is always equal to the number of odd permutations, the signs add up to zero. In the case of figure 1.9 a) the new configurations are depicted in figure 1.11. Now a) represents a double loop generated by placing loops independently, while b) shows a single loop, which is passed twice. Including b) in the allowed single loops ensures the cancelation of forbidden configurations generated by placing loops independently. The same holds true for even more complex structures, such as tripple loops.

If we include the new type of crossings in the loops, then the previous formulas (equation (1.39) [previous page] and equation (1.51) [p. 35]) remain unchanged, with the exception that these crossings also contribute to the number of crossings.

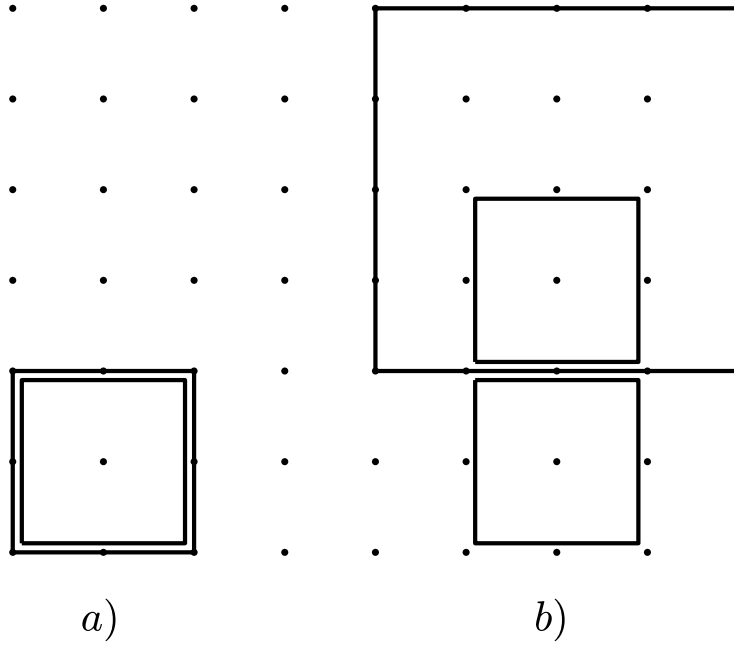


Figure 1.9: *Examples of configurations that occur if loops are placed independently. Such configurations are no valid graphs \tilde{G} .*

Counting then number of loops and corresponding crossing

The remaining task is the determination of D_l , which includes the task of counting the crossings. To this end we introduce directed paths. The n -th step of the path is encoded in

$$S^{(n)} = (\mathbf{x}^{(n)}, \mathbf{d}^{(n)}) \quad (1.42)$$

where $\mathbf{x}^{(n)}$ represents the initial site of the n -th step, and $\mathbf{d}^{(n)} \in \{\pm \mathbf{e}_x, \pm \mathbf{e}_y\}$ the direction of the n -th step. A *path* from $S^{(0)}$ to $S^{(m)}$ is defined by the sequence

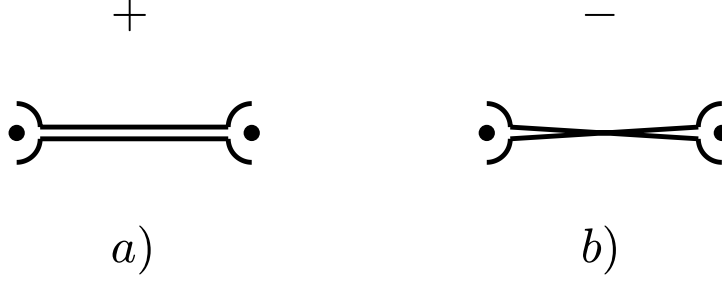
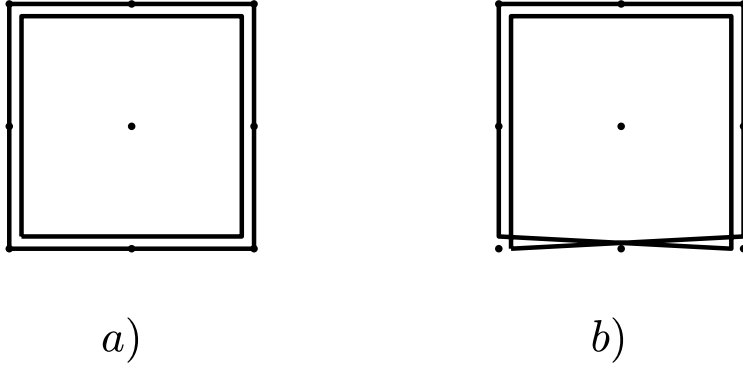
$$\mathcal{P} = S^{(0)}, S^{(1)}, \dots, S^{(m)}$$

Clearly, we have the condition

$$\mathbf{x}^{(n+1)} = \mathbf{x}^{(n)} + \mathbf{d}^{(n)} . \quad (1.43)$$

As the allowed loops do not contain elements that occur when $\mathbf{d}^{(n+1)} = -\mathbf{d}^{(n)}$, we omit such steps. We define the weight of such a path as

$$w(\mathcal{P}) = \prod_{l=1}^m e^{i \frac{1}{2} \Phi(\mathbf{d}^{(l-1)}, \mathbf{d}^{(l)})} , \quad (1.44)$$

Figure 1.10: *Double occupied edges.*Figure 1.11: *Double occupied edges.*

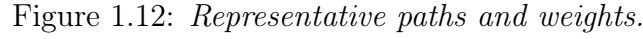
where $\Phi(\mathbf{d}, \mathbf{d}')$ is the angle between the vectors \mathbf{d} and \mathbf{d}' , defined as follows.

$$\Phi(\mathbf{d}, \mathbf{d}') = \begin{cases} 0 & \text{if } \mathbf{d}, \mathbf{d}' \text{ are parallel} \\ \frac{\pi}{2} & \text{if } \mathbf{d}' \text{ is anti-clockwise rotated from } \mathbf{d} \\ -\frac{\pi}{2} & \text{if } \mathbf{d}' \text{ is clockwise rotated from } \mathbf{d} \\ \text{forbidden} & \text{if } \mathbf{d}, \mathbf{d}' \text{ are anti-parallel} \end{cases} \quad (1.45)$$

In figure 1.12 some examples of allowed loops (paths) are given, for which we want to compute the weight. We start at the lower left corner and follow the arrow. We recall that turning left at a vertex gives $+\frac{\pi}{2}$, a right turn $-\frac{\pi}{2}$ and crossing straight adds zero. In subfigure a) the 4 angles Φ encountered during the path are all $\pi/2$. The four angles add up to 2π . In other words we have performed four left turns. The weight is then

$$w = e^{i\frac{1}{2}2\pi} = -1.$$

For example b) the angles are in units of $\frac{\pi}{2}$: 1, 0, -1, -1, -1, 0, 1, 1, with a sum of 0 and a weight $w = +1$. In other words the number of left and right


$$w(\mathcal{P}) = -(-1)^{N_c(L)},$$

Now we define a matrix \mathcal{M} with matrix elements

$$\langle S'|M_m|S\rangle = \sum_{S''} \langle S'|M_{m_1}|S''\rangle \langle S''|M_{m_2}|S\rangle ,$$
$$\mathcal{M}_m = (\mathcal{M}_1)^m.$$

We can now easily express the sought-for weight D_m as

$$D_m = -\frac{1}{2m} \sum_S \langle S | \mathcal{M}_m | S \rangle = -\frac{1}{2m} \text{tr} \{ \mathcal{M}_1^m \}$$

prove

1. The trace is required to sum over all initial vertices of the loop and to make sure that the loop is really closed
2. Since each vertex of a loop occurs as initial point in the trace, we have to divide by m
3. Each loop can be traversed in two direction, which explains the factor $1/2$.
4. The minus sign has been explained before.

q.e.d. ✓

In total we therefore have according to equation (1.51) [\[p. 35\]](#)

$$\begin{aligned}
 \ln(Z) &= N \ln(2) + 2N \ln(\cosh(j)) + \sum_{m=1} D_m t^m \\
 &= N \ln(2) + 2N \ln(\cosh(j)) - \frac{1}{2} \text{tr} \left\{ \sum_{m=1} \frac{(t\mathcal{M}_1)^m}{m} \right\} \\
 &= N \ln(2) + 2N \ln(\cosh(j)) + \frac{1}{2} \text{tr} \{ \ln(\mathbf{1} - t\mathcal{M}_1) \} \\
 &= N \ln(2) + 2N \ln(\cosh(j)) + \frac{1}{2} \ln \det[(\mathbf{1} - t\mathcal{M}_1)] .
 \end{aligned}$$

As said before, the size of the matrix \mathcal{M}_1 is $4N \times 4N$. The matrix elements are defined via

$$\langle \mathbf{x}, \mathbf{d} | \mathcal{M}_1 | \mathbf{x}', \mathbf{d}' \rangle .$$

Since we use pbc, it is advantageous to perform a Fourier transform with respect to \mathbf{x} and \mathbf{x}' . The determinant is invariant against such a unitary transformation. Moreover, due to translational invariance of the problem,

we obtain

$$\begin{aligned}
\langle \mathbf{q}, \mathbf{d} | \mathcal{M}_1 | \mathbf{q}', \mathbf{d}' \rangle &= \frac{1}{N} \sum_{\mathbf{x}, \mathbf{x}'} e^{-i(\mathbf{x} \cdot \mathbf{q} - \mathbf{x}' \cdot \mathbf{q}')} \langle \mathbf{0}, \mathbf{d} | \mathcal{M}_1 | \underbrace{\mathbf{x}' - \mathbf{x}}_{\Delta \mathbf{x}}, \mathbf{d}' \rangle \\
&= \frac{1}{N} \sum_{\mathbf{x}} \underbrace{e^{-i\mathbf{x} \cdot (\mathbf{q} - \mathbf{q}')} }_{=\delta_{\mathbf{q}\mathbf{q}'}} \sum_{\Delta \mathbf{x}} e^{i\mathbf{q}' \cdot \Delta \mathbf{x}} \langle \mathbf{0}, \mathbf{d} | \mathcal{M}_1 | \Delta \mathbf{x}, \mathbf{d}' \rangle \\
&= \delta_{\mathbf{q}\mathbf{q}'} \sum_{\Delta \mathbf{x}} e^{i\mathbf{q} \cdot \Delta \mathbf{x}} \langle \mathbf{0}, \mathbf{d} | \mathcal{M}_1 | \Delta \mathbf{x}, \mathbf{d}' \rangle .
\end{aligned}$$

According to equation (1.43) [p. 28] we have the condition

$$\begin{aligned}
\mathbf{x}' &= \mathbf{x} + \mathbf{d} \\
\Rightarrow \quad \Delta \mathbf{x} &= \mathbf{x}' - \mathbf{x} = \mathbf{d} .
\end{aligned}$$

Hence the 4×4 matrix $M(\mathbf{q})$ has the matrix elements

$$\begin{aligned}
\langle \mathbf{q}, \mathbf{d} | \mathcal{M}_1 | \mathbf{q}', \mathbf{d}' \rangle &= \delta_{\mathbf{q}\mathbf{q}'} e^{i\mathbf{q} \cdot \mathbf{d}} \langle \mathbf{0}, \mathbf{d} | \mathcal{M}_1 | \mathbf{d}, \mathbf{d}' \rangle \\
&= \delta_{\mathbf{q}\mathbf{q}'} \underbrace{e^{i\mathbf{q} \cdot \mathbf{d}} e^{i\frac{1}{2}\Phi(\mathbf{d}, \mathbf{d}')}}_{=M_{\mathbf{d}, \mathbf{d}'}}
\end{aligned}$$

The inverse transformation is

$$\langle \mathbf{x}, \mathbf{d} | \mathcal{M}_1 | \mathbf{x}', \mathbf{d}' \rangle = \frac{1}{N} \sum_{\mathbf{q}} e^{i(\mathbf{x} - \mathbf{x}') \cdot \mathbf{q}} \langle \mathbf{q}, \mathbf{d} | \mathcal{M}_1 | \mathbf{q}, \mathbf{d}' \rangle ,$$

and, therefore,

$$\begin{aligned}
\langle \mathbf{x}, \mathbf{d} | \mathcal{M}^n | \mathbf{x}', \mathbf{d}' \rangle &= \frac{1}{N} \sum_{\mathbf{q}} e^{i(\mathbf{x} - \mathbf{x}') \cdot \mathbf{q}} \langle \mathbf{q}, \mathbf{d} | (\mathcal{M}_1)^n | \mathbf{q}, \mathbf{d}' \rangle \\
&= \frac{1}{N} \sum_{\mathbf{q}} e^{i(\mathbf{x} - \mathbf{x}') \cdot \mathbf{q}} \left((M(\mathbf{q}))^n \right)_{\mathbf{d}, \mathbf{d}'} .
\end{aligned}$$

The remaining 4×4 matrix $M(\mathbf{q})$ has the matrix elements

$$M(\mathbf{q}): \quad \begin{array}{c|cccc} \mathbf{d} \backslash \mathbf{d}' & \mathbf{e}_x & -\mathbf{e}_x & \mathbf{e}_y & -\mathbf{e}_y \\ \hline \mathbf{e}_x & e^{iq_1} & 0 & \lambda e^{iq_1} & \lambda^* e^{iq_1} \\ -\mathbf{e}_x & 0 & e^{-iq_1} & \lambda^* e^{-iq_1} & \lambda e^{-iq_1} \\ \mathbf{e}_y & \lambda^* e^{iq_2} & \lambda e^{iq_2} & e^{iq_2} & 0 \\ -\mathbf{e}_y & \lambda e^{-iq_2} & \lambda^* e^{-iq_2} & 0 & e^{-iq_2} \end{array}$$

with the definition $\lambda = e^{i\frac{\pi}{4}}$. This can also be written as

$$M(\mathbf{q}) = D(\mathbf{q})\tilde{M} \quad (1.46a)$$

$$D(\mathbf{q}) = \text{diag}[e^{iq_1}, e^{-iq_1}, e^{iq_2}, e^{-iq_2}] \quad (1.46b)$$

$$\tilde{M} = \begin{pmatrix} 1 & 0 & \lambda, \lambda^* \\ 0 & 1 & \lambda^*, \lambda \\ \lambda^*, \lambda & 1 & 0 \\ \lambda, \lambda^* & 0 & 1 \end{pmatrix} \quad (1.46c)$$

Here \tilde{M} is a hermitean matrix but M is not. As the matrix is blockdiagonal in \mathbf{q}, \mathbf{q}' we have

$$\det(\mathbf{1} - t\mathcal{M}_1) = \det(t\mathcal{M}_1 - \mathbf{1}) = \prod_{\mathbf{q}}^{1bc} \det(tM(\mathbf{q}) - \mathbf{1})$$

With $Q_\alpha = te^{iq_\alpha}$ the matrix argument of the determinant reads

$$tM(\mathbf{q}) - \mathbf{1} = - \begin{pmatrix} Q_1 - 1 & 0 & \lambda Q_1 & \lambda^* Q_1 \\ 0 & Q_1^* - 1 & \lambda^* Q_1^* & \lambda Q_1^* \\ \lambda^* Q_2 & \lambda Q_2 & Q_2 - 1 & 0 \\ \lambda Q_2^* & \lambda^* Q_2^* & 0 & Q_2^* - 1 \end{pmatrix}.$$

The determinant yields (according to MATHEMATICA)

$$\ln \left[\det(\mathbf{1} - t\mathcal{M}_1) \right] = \sum_{\mathbf{q}}^{1bc} \ln \left[(1 + t^2)^2 - 2t(1 - t^2)(\cos(q_1) + \cos(q_2)) \right].$$

Then the free energy per site is

$$-\beta \frac{F}{N} = \ln(2) + 2 \ln(\cosh(j)) + \frac{1}{2N} \sum_{\mathbf{q}}^{1bc} \ln \left[(1 + t^2)^2 - 2t(1 - t^2)(\cos(q_1) + \cos(q_2)) \right] \quad (1.47)$$

We introduce the normalized density of states $\rho(\varepsilon)$ corresponding to the dispersion

$$\varepsilon(\mathbf{q}) = -(\cos(q_1) + \cos(q_2)) \quad (1.48)$$

$$\rho(\varepsilon) = \frac{1}{N} \sum_{\mathbf{q}}^{1bc} \delta(\varepsilon(\mathbf{q}) - \varepsilon) \quad (1.49)$$

$$-\beta \frac{F}{N} = \ln(2) + 2 \ln(\cosh(j)) + \frac{1}{2} \int d\varepsilon \rho(\varepsilon) \ln \left[(1+t^2)^2 + 2t(1-t^2) \varepsilon \right]. \quad (1.50)$$
$$\begin{aligned} \cosh(j) &= \frac{1}{\sqrt{1-t^2}}, \quad (t := \tanh(j)) \\ 2 \ln(\cosh(j)) &= \frac{1}{2} \ln((1-t^2)^{-2}) = \frac{1}{2} \int d\varepsilon \, \rho(\varepsilon) \ln((1-t^2)^{-2}) \end{aligned}$$
$$\begin{aligned} -\beta \frac{F}{N} &= \ln(2) + \frac{1}{2} \int d\varepsilon \rho(\varepsilon) \ln \left[\left(\frac{1+t^2}{1-t^2} \right)^2 + \left(\frac{2t}{1-t^2} \right) \varepsilon \right] \\ &= \ln(2) + \frac{1}{2} \int d\varepsilon \rho(\varepsilon) \ln \left[\underbrace{\left(\frac{1+t^2}{1-t^2} \right)^2 - \left(\frac{4t}{1-t^2} \right)}_{=\left(1-\sinh(2j)\right)^2} + \underbrace{\left(\frac{2t}{1-t^2} \right)}_{=\sinh(2j)} (2+\varepsilon) \right]. \end{aligned}$$
$$\begin{aligned} \frac{2t}{1-t^2} &= \frac{2 \tanh(j)}{1 - \tanh^2(j)} \\ &= \frac{2sh/ch}{\underbrace{(ch^2 - sh^2)}_{=1}/ch^2} \\ &= 2 \sinh(j) \cosh(j) = \sinh(2j) \\ &\quad \textcolor{blue}{=\cosh(2j)} \\ \left(\frac{4t}{1-t^2} \right) &= \left(\underbrace{\frac{ch^2 + sh^2}{ch^2 - sh^2}}_{=1} \right)^2 - \underbrace{\left(2 \frac{2t}{1-t^2} \right)}_{=2 \sinh(2j)} \\ &= \cosh^2(2j) - 2 \sinh(2j) \\ &= 1 + \sinh^2(2j) - 2 \sinh(2j) \\ &= \left(1 - \sinh(2j) \right)^2 . \end{aligned}$$

q.e.d. ✓

The final result for the free energy reads thereore

<p>FREE ENERGY OF THE 2D ISING MODEL (without external field)</p> <hr style="border: 0.5px solid black;"/> $\frac{\ln(Z)}{N} = -\beta \frac{F}{N} = \ln(2) + \frac{1}{2} \int d\varepsilon \rho(\varepsilon) \ln \left[(1 - \sinh(2j))^2 + \sinh(2j) (2 + \varepsilon) \right].$ <p style="text-align: right;">(1.51)</p>
--

It is to be remembered that $j = J\beta > 0$ for the ferromagnetic model. Therefore, $\sinh(2j) > 0$. According to equation (1.48) [p. 33], the energies ε are restricted to the interval $[-2, 2]$. The density of states $\rho(\varepsilon)$ is that of the 2d tight binding model, which is given by

$$\rho(\varepsilon) = \frac{\theta(|\varepsilon| \leq 2)}{2\pi^2} \mathcal{K} \left(1 - \left(\frac{\varepsilon}{2} \right)^2 \right), \quad (1.52)$$

where $\mathcal{K}(x)$ is the elliptic integral of the first kind

$$\mathcal{K}(x) = \int_0^{\frac{\pi}{2}} \frac{d\varphi}{\sqrt{1 - x^2(\sin \varphi)^2}}. \quad (1.53)$$

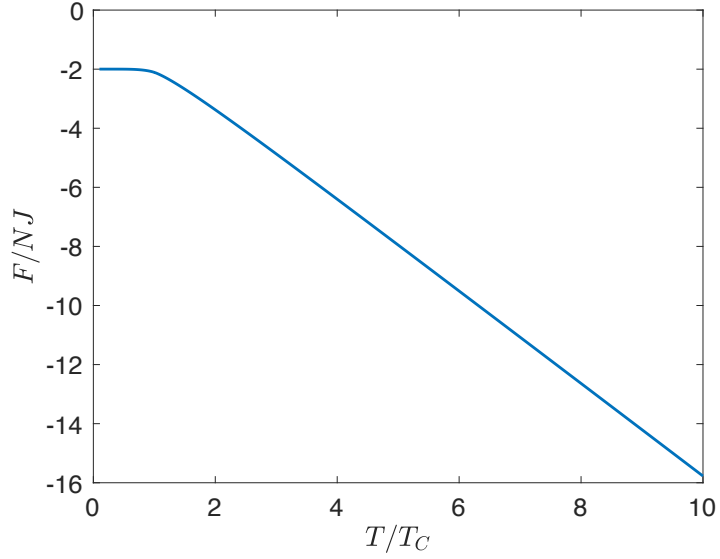
The free energy is related to the entropy and internal energy through

$$F = U - TS.$$

As we will easily see later on, for $T \rightarrow 0$ we have $U \rightarrow -2JN$ and $S \rightarrow 0$ (3. law of thermodynamics), hence $F \rightarrow -2JN$; while for $k_B T/J \gg 1$ we have $U \rightarrow 0$ and $S \rightarrow Nk_B \ln(2)$, hence $F \rightarrow -Nk_B T \ln(2)$.

1.3.5 Curie-temperature

If we would have computed the free energy in the presence of an external magnetic field, we could have computed the magnetization and from that directly the transition temperature. In the absence of an external field, the

Figure 1.13: *Free energy of the 2D Ising model.*

magnetization is always zero, due to symmetry. But in order to allow for a phase transition the free energy has to have an irregularity. (The argument will be given later.) The argument of the logarithm is non-negative, but it can be zero which yields the required irregularity. For the argument to become zero, both terms $(1 - \sinh(2j))^2$ and $\sinh(2j)(2 + \varepsilon)$ have to be zero. The first condition yields

$$\sinh(2j_C) = 1 \quad (1.54)$$

$$\begin{aligned} 1 - \sinh(2j) &= 1 - \frac{e^{2j_C} + e^{-2j_C}}{2} = 0 \\ \Rightarrow e^{2j_C} + e^{-2j_C} - 2 &= 0 \\ e^{4j_C} - 2e^{2j_C} + 1 &= 0. \end{aligned}$$

This quadratic equation has the solutions

$$e^{2j_C} = 1 \pm \sqrt{2}.$$

Since $e^{2j} > 0$ the only solution is

$$j_C = J\beta_C = \frac{1}{2} \ln(1 + \sqrt{2}) = 0.4407. \quad (1.55)$$

The mean field result was $J\beta_C = 0.25$. The irregularity of the free energy is a necessary prerequisite for phase transition, but not sufficient for a rigorous prove. Nor does it tell us the order of the phase transition. The rigorous prove requires the dependence of the free energy on the an external field.

1.3.6 Internal energy

$$U = \langle H \rangle = -J \sum_{\langle ij \rangle} \langle S_i S_j \rangle .$$

Due to the translational invariance all n.n. correlations are the same

$$\frac{U}{NJ} = -2 \langle S_1 S_2 \rangle .$$

For high temperatures the spins are uncorrelated resulting in

$$\frac{U}{NJ} = -2 \langle S_1 \rangle \langle S_2 \rangle = 0 ,$$

while for $T = 0$, the lowest energy is obtained if all spins are parallel and

$$\frac{U}{NJ} = -2 .$$

Now we compute U for arbitrary temperature. To this end, we write $\ln(Z)$ in a more compact form

$$\ln(Z) = \ln(2) + \frac{1}{2} \underbrace{\left\langle \ln \left((1 - \kappa)^2 + \kappa(2 + \varepsilon) \right) \right\rangle}_{=g(\kappa)} ,$$

the average here is taken w.r.t. $\rho(\varepsilon)$, and $\kappa = \sinh(2\beta J)$. Then

$$\begin{aligned} \frac{U}{N} &= \frac{\langle H \rangle}{N} = -\frac{\partial \ln(Z)}{\partial \beta} \\ &= -\frac{1}{2} \left(\frac{\partial}{\partial \kappa} g(\kappa) \right) \frac{d\kappa}{d\beta} . \end{aligned}$$

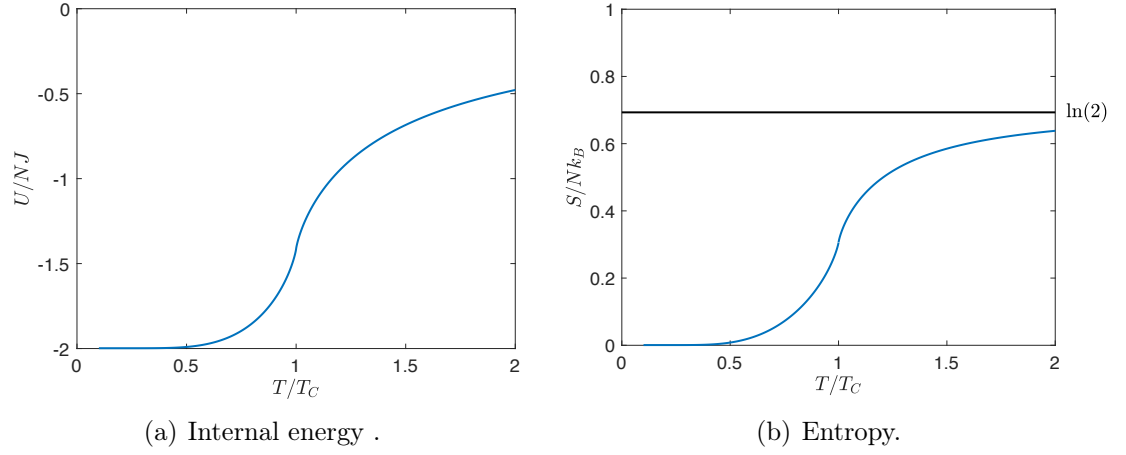
with

$$\frac{\partial \kappa}{\partial \beta} = \frac{\partial}{\partial \beta} \sinh(2J\beta) = 2J \cosh(2J\beta) = 2J \sqrt{1 + \sinh^2(2J\beta)}$$

we have

$$\begin{aligned} \frac{U}{N} &= -J g'(\kappa) \sqrt{1 + \kappa^2} \\ &= -J \left\langle \frac{2\kappa + \varepsilon}{(1 - \kappa)^2 + \kappa(2 + \varepsilon)} \right\rangle \sqrt{1 + \kappa^2} . \end{aligned}$$

In summary we have

Figure 1.14: *2d Ising model for $B = 0$.*

INTERNAL ENERGY	
$\frac{U}{NJ} = - \left\langle \frac{2\kappa + \varepsilon}{(1 - \kappa)^2 + \kappa(2 + \varepsilon)} \right\rangle \sqrt{1 + \kappa^2} .$	(1.56)

1.3.7 Entropy

From $F = U - TS$ we get

$$\frac{S}{Nk_B} = j \frac{U}{NJ} - \beta \frac{F}{N} = j \left(\frac{U}{NJ} \right) + \left(\frac{\ln(Z)}{N} \right) .$$

Hence, we can express the entropy in terms of equation (1.56) and equation (1.51) [p. 35].

We see no critical behaviour in the entropy, which is the first derivative of the free energy w.r.t. T . The latter is continuous at T_C . According to [section \(5.2.3\)](#) [Seite 122] it is therefore not a first order phase transition.

1.3.8 Specific heat

The order of the phase transition can also be inferred from the specific heat at $B = 0$.

$$\begin{aligned} \frac{C}{N} &= \frac{1}{N} \frac{\partial U}{\partial T} \Big|_N = \frac{1}{N} \frac{\partial U}{\partial \kappa} \underbrace{\frac{\partial \kappa}{\partial \beta}}_{=2J\sqrt{1+\kappa^2} = -\frac{1}{k_B T^2}} \underbrace{\frac{\partial \beta}{\partial T}} \\ &= \left[\frac{\partial}{\partial \kappa} \left(-Jg'(\kappa)\sqrt{1+\kappa^2} \right) \right] \left(-k_B \beta^2 (2J\sqrt{1+\kappa^2}) \right) \end{aligned}$$

The final result reads

$$\frac{C(T)}{Nk_B} = 2j^2 \left[(1+\kappa^2)g''(\kappa) + \kappa g'(\kappa) \right]. \quad (1.57a)$$

with

$$g'(\kappa) = \left\langle \frac{2\kappa + \varepsilon}{(1-\kappa)^2 + \kappa(2+\varepsilon)} \right\rangle \quad (1.57b)$$

$$g''(\kappa) = \left\langle \frac{2}{(1-\kappa)^2 + \kappa(2+\varepsilon)} \right\rangle - \left\langle \left(\frac{2\kappa + \varepsilon}{(1-\kappa)^2 + \kappa(2+\varepsilon)} \right)^2 \right\rangle \quad (1.57c)$$

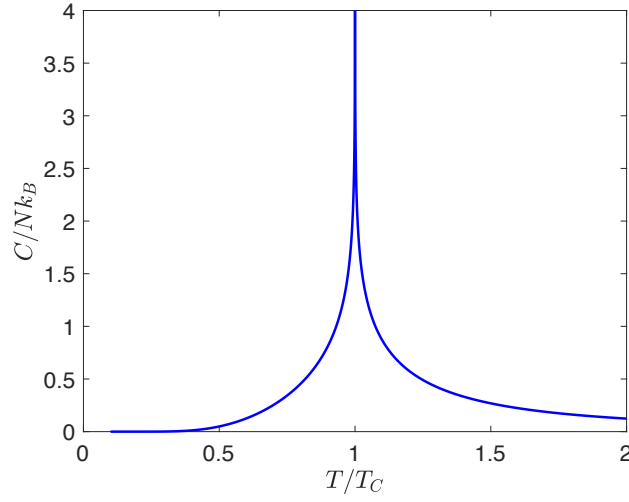
We see in figure 1.15 that the specific heat diverges at T_C . In order to unravel the type of divergency we perform a Taylor expansion in T about T_C , i.e. $T = T_C + \Delta T$. This corresponds to

$$\begin{aligned} j &= j_C + \Delta j \\ \kappa &= \sinh(2J_C + \Delta\kappa) = 1 + \Delta\kappa \end{aligned}$$

In the last step we have used equation (1.54) [p. 36]. The only divergent behaviour can come from g' or g'' . The other terms can, therefore, be replaced by $T = T_C$. I.e.

$$\frac{C(T_C + \Delta T)}{Nk_B} = 2j_C^2 \left[2g''(\kappa_c + \Delta\kappa) + g'(\kappa_c + \Delta\kappa) \right].$$

There is a critical behaviour in the second derivative of F , i.e. the specific heat. Therefore, the Ising model has [a second order phase transition](#).

Figure 1.15: *Specific heat of the 2d Ising model.*

Type of divergency

The divergency originates from the term $\frac{1}{(1-\kappa)^2 + \kappa(\varepsilon+2)}$ at the vicinity of $\varepsilon = -2$. The dos $\rho(\varepsilon)$ in principle also has a divergency at $\varepsilon = 0$ but it is integrable and does not result in a divergency in the specific heat. To study the divergency at $\varepsilon = -2$ we split

$$\rho(\varepsilon) = \underbrace{\rho(-2)}_{=\rho_0} + \Delta\rho(\varepsilon) .$$

Then the expectation values become

$$\langle F(\varepsilon) \rangle = \langle F(\varepsilon) \rangle_{\rho_0} + \langle F(\varepsilon) \rangle_{\Delta\rho} .$$

The second term cause no divergency, hence we merely need to consider terms of the form

$$\langle F(\varepsilon) \rangle_{\rho_0} . \tag{1.58}$$

$$\begin{aligned}
& \lim_{\varepsilon \rightarrow -2} \frac{\Delta\rho(\varepsilon)(2 + \varepsilon + 2\Delta\kappa)}{(\Delta\kappa)^2 + (1 + \Delta\kappa)(\varepsilon + 2)} \\
&= \lim_{\eta \rightarrow 0} \frac{\Delta\rho(-2 + \eta)(\eta + 2\Delta\kappa)}{(\Delta\kappa)^2 + (1 + \Delta\kappa)\eta} \\
&\stackrel{L'Hospital}{=} \lim_{\eta \rightarrow 0} \frac{\Delta\rho'(-2 + \eta)(\eta + 2\Delta\kappa) + \Delta\rho(-2 + \eta)}{(\Delta\kappa)^2 + (1 + \Delta\kappa)\eta} \\
&= \lim_{\eta \rightarrow 0} \frac{(2\Delta\kappa\Delta\rho'(-2 + \eta) + \Delta\rho(-2 + \eta))}{(\Delta\kappa)^2} \\
&= \frac{2}{\Delta\kappa} \lim_{\eta \rightarrow 0} \underbrace{\Delta\rho'(-2 + \eta)}_{=0} + \frac{1}{(\Delta\kappa)^2} \lim_{\eta \rightarrow 0} \underbrace{\Delta\rho(-2 + \eta)}_{=0} \\
&= 0 .
\end{aligned}$$

or for g'' we need

$$\begin{aligned}
& \lim_{\varepsilon \rightarrow -2} \Delta\rho(\varepsilon) \left(\frac{2 + \varepsilon + \Delta\kappa}{(\Delta\kappa)^2 + (1 + \Delta\kappa)(\varepsilon + 2)} \right)^2 \\
&= \lim_{\eta \rightarrow 0} \frac{\Delta\rho(-2 + \eta)(\eta + \Delta\kappa)^2}{((\Delta\kappa)^2 + (1 + \Delta\kappa)\eta)^2} \\
&\stackrel{L'Hospital}{=} \lim_{\eta \rightarrow 0} \frac{\Delta\rho'(-2 + \eta)(\eta + \Delta\kappa)^2 + 2\Delta\rho(-2 + \eta)(\eta + \Delta\kappa)}{2((\Delta\kappa)^2 + (1 + \Delta\kappa)\eta)(1 + \Delta\kappa)} \\
&\stackrel{L'Hospital}{=} \lim_{\eta \rightarrow 0} \frac{\Delta\rho'(-2 + \eta)(\Delta\kappa)^2 + 2\Delta\kappa\Delta\rho(-2 + \eta)}{2((\Delta\kappa)^2)(1 + \Delta\kappa)} \\
&= \frac{(\Delta\kappa)^2}{2((\Delta\kappa)^2)(1 + \Delta\kappa)} \lim_{\eta \rightarrow 0} \underbrace{\Delta\rho'(-2 + \eta)}_{=0} + \frac{2\Delta\kappa}{2((\Delta\kappa)^2)(1 + \Delta\kappa)} \lim_{\eta \rightarrow 0} \underbrace{\Delta\rho(-2 + \eta)}_{=0} \\
&= 0 .
\end{aligned}$$

q.e.d. ✓

For the first term in equation (1.57) [p. 39] we need

$$g'(1 + \Delta\kappa) = \left\langle \frac{\varepsilon + 2 + \Delta\kappa}{(2 + \varepsilon)(1 + \Delta\kappa) + (\Delta\kappa)^2} \right\rangle_{\rho_0} ,$$

for which we find

$$\begin{aligned} g'(1 + \Delta\kappa) &= \frac{1}{1 + \Delta\kappa} \cdot \{4\rho_0 + \Delta\kappa\rho_0 \ln(4) - 2\rho_0\Delta\kappa \ln(\Delta\kappa) + O(\Delta\kappa)\} \\ &\xrightarrow{\Delta\kappa \rightarrow 0} 4\rho_0 = O(1) . \end{aligned}$$

Proof

First we will transform the denominator

$$\begin{aligned} (2 + \varepsilon)(1 + \Delta\kappa) + (\Delta\kappa)^2 &= (1 + \Delta\kappa) \left(2 + \varepsilon + \frac{(\Delta\kappa)^2}{1 + \Delta\kappa} \right) \\ &= (1 + \Delta\kappa) \left(2 + \varepsilon + (\Delta\kappa)^2 + O((\Delta\kappa)^3) \right) \end{aligned}$$

Then

$$\begin{aligned} &\frac{\varepsilon + 2 + \Delta\kappa}{(2 + \varepsilon)(1 + \Delta\kappa) + (\Delta\kappa)^2} \\ &= \frac{1}{1 + \Delta\kappa} \cdot \frac{\varepsilon + 2 + \Delta\kappa}{2 + \varepsilon + (\Delta\kappa)^2 + O((\Delta\kappa)^3)} \\ &= \frac{1}{1 + \Delta\kappa} \cdot \frac{\varepsilon + 2 + (\Delta\kappa)^2 + O((\Delta\kappa)^3) + \Delta\kappa(1 - \Delta\kappa) + O((\Delta\kappa)^3)}{2 + \varepsilon + (\Delta\kappa)^2 + O((\Delta\kappa)^3)} . \end{aligned}$$

I.e.

$$\frac{\varepsilon + 2 + \Delta\kappa}{(2 + \varepsilon)(1 + \Delta\kappa) + (\Delta\kappa)^2} = \frac{1}{1 + \Delta\kappa} \cdot \left\{ 1 + \frac{\Delta\kappa(1 - O((\Delta\kappa)^2))}{2 + \varepsilon + (\Delta\kappa)^2(1 + O(\Delta\kappa))} \right\} . \quad (1.59)$$

So we have

$$\begin{aligned} g'(1 + \Delta\kappa) &= \left\langle \frac{\varepsilon + 2 + \Delta\kappa}{(2 + \varepsilon)(1 + \Delta\kappa) + (\Delta\kappa)^2} \right\rangle_{\rho_0} \\ &= \frac{1}{1 + \Delta\kappa} \cdot \left\{ \langle 1 \rangle_{\rho_0} + \Delta\kappa(1 - O((\Delta\kappa)^2)) \left\langle \frac{1}{2 + \varepsilon + (\Delta\kappa)^2(1 + O(\Delta\kappa))} \right\rangle_{\rho_0} \right\} \end{aligned}$$

The definition of the expectation value is

$$\langle f(\varepsilon) \rangle_{\rho_0} := \int_{-2}^2 f(\varepsilon) \rho_0 d\varepsilon = \rho_0 \int_{-2}^2 f(\varepsilon) d\varepsilon .$$

Therefore

$$\langle 1 \rangle_{\rho_0} = 4\rho_0 .$$

$$\begin{aligned} & \left\langle \frac{1}{2 + \varepsilon + (\Delta\kappa)^2(1 + O(\Delta\kappa))} \right\rangle_{\rho_0} \\ &= \rho_0 \int_{-2}^2 \frac{1}{2 + \varepsilon + (\Delta\kappa)^2(1 + O(\Delta\kappa))} d\varepsilon \\ &= \rho_0 \ln \left(2 + 2 + (\Delta\kappa)^2(1 + O(\Delta\kappa)) \right) - \rho_0 \ln \left(2 - 2 + (\Delta\kappa)^2(1 + O(\Delta\kappa)) \right) \\ &= \rho_0 \ln(4) - \rho_0 \ln((\Delta\kappa)^2) + O(\Delta\kappa) \end{aligned}$$

In total we have

$$\begin{aligned} g'(1 + \Delta\kappa) &= \left\langle \frac{\varepsilon + 2 + \Delta\kappa}{(2 + \varepsilon)(1 + \Delta\kappa) + (\Delta\kappa)^2} \right\rangle_{\rho_0} \\ &= \frac{1}{1 + \Delta\kappa} \cdot \{4\rho_0 + \Delta\kappa\rho_0 \ln(4) - 2\rho_0\Delta\kappa \ln(\Delta\kappa) + O(\Delta\kappa)\} \\ &\xrightarrow{\Delta\kappa \rightarrow 0} 0 . \end{aligned}$$

q.e.d. ✓

Similarly, for the second term of g'' we find with equation (1.59) [\[previous page\]](#)

$$\begin{aligned} & \left\langle \left(\frac{2\kappa + \varepsilon}{(1 - \kappa)^2 + \kappa(2 + \varepsilon)} \right)^2 \right\rangle_{\rho_0} \\ &= \left(\frac{1}{1 + \Delta\kappa} \right)^2 \cdot \left\langle \left(1 + \frac{\Delta\kappa(1 - O((\Delta\kappa)^2))}{2 + \varepsilon + (\Delta\kappa)^2(1 + O(\Delta\kappa))} \right)^2 \right\rangle_{\rho_0} \\ &= O(1) + O(\Delta\kappa \ln(\Delta\kappa)) + O((\Delta\kappa)^2) \int_{-2}^2 \frac{1}{2 + \varepsilon + (\Delta\kappa)^2} d\varepsilon \\ &= O(1) + O(\Delta\kappa \ln(\Delta\kappa)) + O((\Delta\kappa)^2) \left(O(1) + O\left(\frac{1}{(\Delta\kappa)^2}\right) \right) \\ &= O(\Delta\kappa \ln(\Delta\kappa)) + O(1) + O((\Delta\kappa)^2) \end{aligned}$$

Again no divergency. The only divergent term stems from the first part of g'' , which yields

$$\begin{aligned}
 \left\langle \frac{2}{(\Delta\kappa)^2 + (1 + \Delta\kappa)(2 + \varepsilon)} \right\rangle_{\rho_0} &= \int_{-2}^2 \frac{\rho_0}{(\Delta\kappa)^2 + (1 + \Delta\kappa)(2 + \varepsilon)} d\varepsilon \\
 &= \rho_0 \ln [(\Delta\kappa)^2 + (1 + \Delta\kappa)(2 + 2)] - \rho_0 \ln [(\Delta\kappa)^2 + (1 + \Delta\kappa)(2 - 2)] \\
 &= \rho_0 \ln [4 + O(\Delta\kappa)] - 2\rho_0 \ln(|\Delta\kappa|); \\
 &= O(1) - 2 \ln(|\Delta\kappa|);
 \end{aligned}$$

The specific heat obviously has a logarithmic divergency, which corresponds to the critical exponent

$$\alpha = \alpha' = 0 . \quad (1.60)$$

For the definition of the critical exponents see [section \(5.3\)](#) [[Seite 123](#)].

1.3.9 Spontaneous magnetization

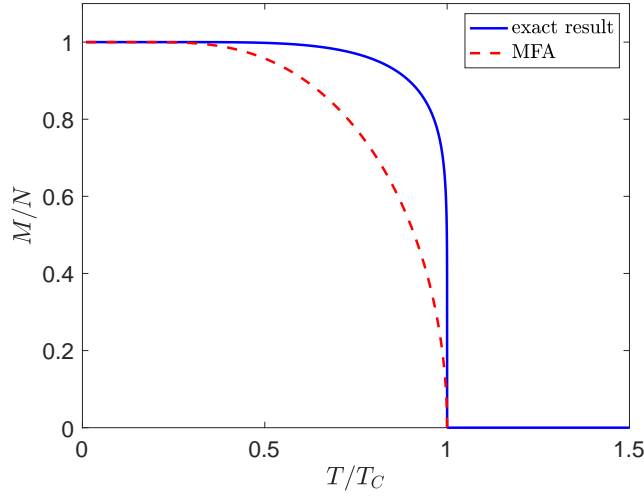
So far it has not been possible to find the exact solution of the 2d Ising model in an external magnetic field. This is only doable for infinitesimal B values, which is enough to determine the spontaneous magnetization. It amounts to computing the spin-spin correlation $\langle S_i S_j \rangle$ and use

$$\lim_{l \rightarrow \infty} \langle S_i S_{i+l} \rangle \longrightarrow \left(\langle S_i \rangle \right)^2 = \left(\frac{M}{N} \right)^2 .$$

The graphical solution amounts to count all graphs as before but with the peculiarity that the vertices i and j have an odd order. The result reads

SPONTANEOUS MAGNETIZATION OF THE 2D ISING MODEL	
$\frac{M}{N} = \begin{cases} (1 - \sinh^{-4}(2j))^{1/8} & \text{for } T \leq T_C \\ 0 & \text{otherwise} \end{cases}$	(1.61)

The order parameter, the magnetization, is continuous, which corroborates the statement, that it is a second order phase transition.

Figure 1.16: *Spontaneous magnetization of Ising spins.*

1.3.10 Proof

We seek the number of paths from the center $\mathbf{x} = 0$ to site \mathbf{x} , where the Manhattan distance is n . We consider only cases with $n > 1$, actually we are interested in $n - 1$ to ∞ . We are interested in the weighted sum over all paths from the center to site \mathbf{x} . Schematically this can be written as

$$Z_{0\mathbf{x}} = \sum_{m=n}^{\infty} W_{0,\mathbf{x}}^{(m)},$$

where $W_{0,\mathbf{x}}^{(m)}$ stands for the contributions that contain m steps. We will again use the previous matrix $M^{(m)}$. Here, however, we are not counting loops and therefore the weights are not entirely correct and it is not yet clear what we have to do with the directions of the last step, which points from the final point \mathbf{x} to an arbitrary direction. It is, therefore, useful, to split off the last step. Then it seems reasonable to start with the form

$$W_{0,\mathbf{x}}^{(m)} = \sum_{\mathbf{d}_0} \sum_{\mathbf{x}', \mathbf{d}'} \left(M^{(m-1)} \right)_{(0,\mathbf{d}_0), (\mathbf{x}', \mathbf{d}')} \left(M^{(1)} \right)_{(\mathbf{x}', \mathbf{d}'), (\mathbf{x}, \mathbf{d}'')}$$

There is one constraint:

$$\mathbf{x}' = \mathbf{x} - \mathbf{d}'.$$

The last term adds a factor $th(j)$ plus a phase, that depends on the yet undefined \mathbf{d}'' . The phase-factors are only correct in closed loops to add up

to the sign, representing crossings. Therefore, we will add graph elements to form a closed loop, such that no additional crossings occur. There are 16 possibilities depending on \mathbf{d} and

vvd'

1.3.11 Critical exponent

For $T \searrow T_C$ we have

$$\begin{aligned} \frac{M}{N} &= \left(1 - [\sinh(2j_C + 2J\Delta\beta)]^{-4} \right)^{\frac{1}{8}} \\ &= \left(1 - \underbrace{[\sinh(2j_C)]}_{\textcolor{blue}{(1,54)}_1} + \cosh(2j_C)J\Delta\beta \right)^{-4} \right)^{\frac{1}{8}}. \end{aligned}$$

In addition, we have

$$\cosh(2j_C) = \sqrt{1 + \sinh^2(2j_C)} = \sqrt{2}.$$

Hence

$$\begin{aligned} \frac{M}{N} &= \left(1 - [1 + \sqrt{2}J\Delta\beta]^{-4} \right)^{\frac{1}{8}} \\ &= \left(1 - 1 + 4\sqrt{2}J\Delta\beta \right)^{\frac{1}{8}} \\ &= \left(4\sqrt{2}J\Delta\beta \right)^{\frac{1}{8}} \\ &= \propto \left(\frac{1}{T} - \frac{1}{T_C} \right)^{\frac{1}{8}} \\ &\propto \varepsilon^{\frac{1}{8}} \end{aligned}$$

Chapter 2

Ising a la Samuel

2.1 Grassmann variables

To allow for all elements for admissible graphs we introduce per site 4 Grassmann variables, two for each direction $h_i^x, h_i^o, v_i^x, v_i^o$, where the first two are for the horizontal direction and the second two for vertical direction. These are 4 independent variables. Let η stand for one of these variables, then they fulfill

$$\begin{aligned}\int d\eta &= 0 \\ \int d\eta \eta &= 1 \\ \eta^2 &= 0\end{aligned}$$

We introduced the trace (tr), which means

$$\text{tr} \{f(\{h_i^x, h_i^o, v_i^x, v_i^o\})\} = \int \dots \int \mathcal{D}_{hv} f(\{h_i^x, h_i^o, v_i^x, v_i^o\}) \quad (2.1a)$$

$$\mathcal{D}_{hv} = \prod_i dh_i^x dh_i^o, dv_i^x, dv_i^o \quad (2.1b)$$

In particular for a single pair of GV at one site we have

$$\int \int dh_i^x dh_i^o h_i^o h_i^x = \underbrace{\int dh_i^x h_i^x}_{=1} \underbrace{\int dh_i^o h_i^o}_{=1} = 1, \quad (2.2)$$

but

$$\int \int dh_i^x dh_i^o h_i^x h_i^o = - \underbrace{\int dh_i^x h_i^x}_{=1} \underbrace{\int dh_i^o h_i^o}_{=1} = -1. \quad (2.3)$$

Obviously, at each site all four GVs have to be present, otherwise the trace over all GVs vanishes.

We introduce the following graphical meaning for the GV

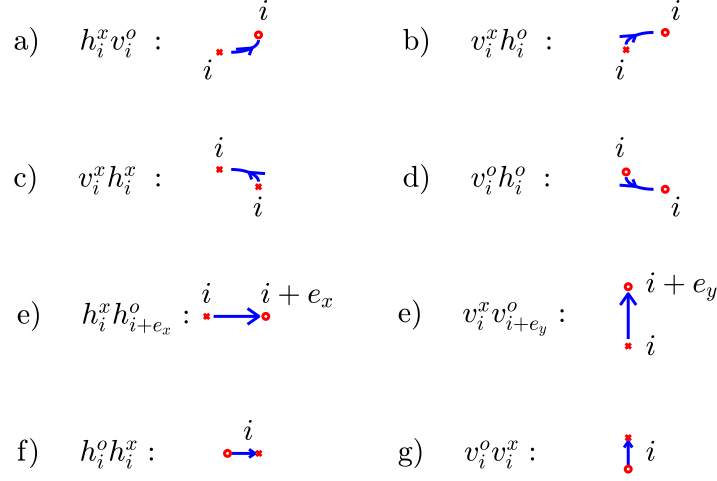


Figure 2.1: *The 6 GV-pairs that form the graph elements.*

Then we introduce an action with theses elements

$$A = A_{\text{bonds}} + A_{\text{corners}} + A_{\text{monomers}} \quad (2.4a)$$

$$A_{\text{bonds}} = t \sum_i \left(h_{\mathbf{x}_i}^x h_{\mathbf{x}_i + \mathbf{e}_x}^o + v_{\mathbf{x}_i}^x v_{\mathbf{x}_i + \mathbf{e}_y}^o \right) \quad (2.4b)$$

$$A_{\text{corners}} = - \sum_i \left(h_{\mathbf{x}_i}^x v_{\mathbf{x}_i}^o + v_{\mathbf{x}_i}^x h_{\mathbf{x}_i}^o + v_{\mathbf{x}_i}^x h_{\mathbf{x}_i}^x + v_{\mathbf{x}_i}^o h_{\mathbf{x}_i}^o \right) \quad (2.4c)$$

$$A_{\text{monomers}} = - \sum_i \left(h_{\mathbf{x}_i}^o h_{\mathbf{x}_i}^x + v_{\mathbf{x}_i}^o v_{\mathbf{x}_i}^x \right) \quad (2.4d)$$

$$A = \sum_{i=1}^N \sum_{\nu=1}^{n_i} P_i^{(\nu)} \quad (2.4e)$$

These elements are depicted in figure 2.1. The reason for the minus signs will be clarified later on. We can then define a kind of partition function

$$Z = \text{tr} e^A .$$

We will show in the sequel that

$$\sum_G t^{N_e(G)} = (-1)^N Z .$$

Since we have a quadratic action in the GVs, we can compute the partition function analytically. Due to the Grassmannian properties, the pair-variables fullfill $P^2 = 0$. When expanding e^A we, therefore, obtain

$$e^A = \prod_{i=1}^N \prod_{\nu=1}^{n_i} (1 + P_i^{(\nu)}) .$$

Each GV-pair is of the form

$$\eta_{i_1}^{\alpha_1} \eta_{i_2}^{\alpha_2} ,$$

where the lower index stand for the site and the upper (type-)index combines the direction $\{h, v\}$ and the flavor $\{x, o\}$. So we can suitably combine the the GV-pairs $P_i^{(\nu)}$. In doing so, we have to keep in mind that each variable for site i , i.e. $\{h_{\mathbf{x}_i}^x, h_{\mathbf{x}_i}^o, v_{\mathbf{x}_i}^x, v_{\mathbf{x}_i}^o\}$ has to occur once and only once.

The graphical elements, required to form admitted graphs, are depicted in figure 2.2. This elements are all that is required to form all admitted graphs; and due to the Grassmannian properties each graph is generated exactly once. Hence, we have essentially

$$\text{tr} \left\{ e^A \right\} = \sum_G \text{sign}(G) t^{N_e(G)} .$$

The factors t are correctly included since each bond is associated with a factor t . We still need to make sure that each admitted graph has the correct sign. In addition, to the sites that have lines attached to them, we also need to ensure that empty site are included correctly, i.e. they should only multiply a factor 1 to each graph.

2.1.1 Monomers

The monomers add missing variables, either for empty sites, or those not used for building the graphs.

Empty sites can be formed by a monomer pair for the horizontal and one for the vertical direction, i.e.

$$h_{\mathbf{x}_i}^o h_{\mathbf{x}_i}^x v_{\mathbf{x}_i}^o v_{\mathbf{x}_i}^x$$

and the trace gives

$$\underbrace{\int \int dh_{\mathbf{x}_i}^x dh_{\mathbf{x}_i}^o h_{\mathbf{x}_i}^o h_{\mathbf{x}_i}^x}_{=1} \cdot \underbrace{\int \int dv_{\mathbf{x}_i}^x dv_{\mathbf{x}_i}^o v_{\mathbf{x}_i}^o v_{\mathbf{x}_i}^x}_{=1} = 1 .$$

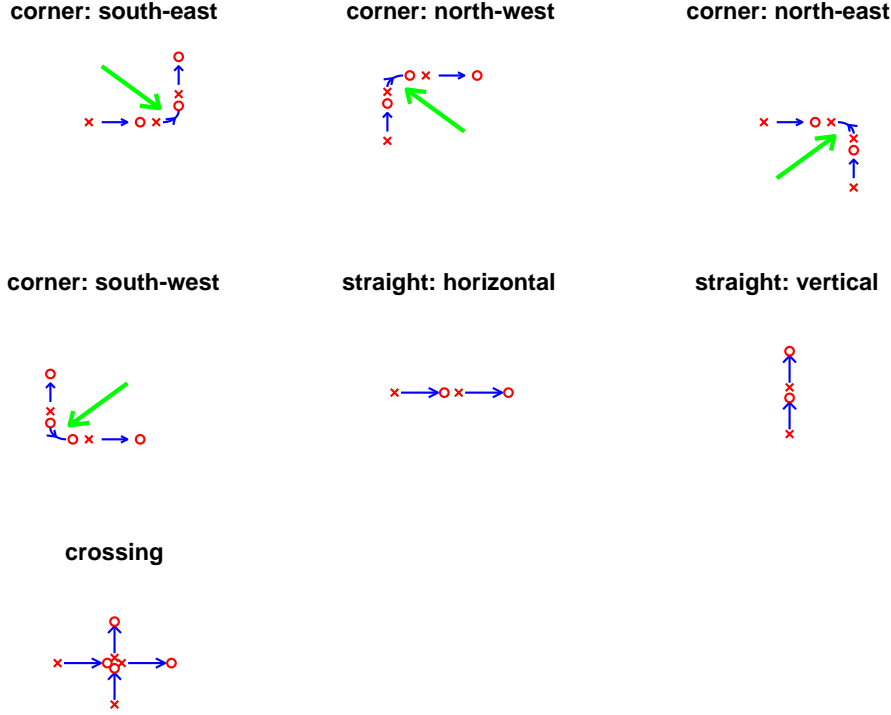


Figure 2.2: All possible combinations of GV-pairs at one site. Monomers that form empty sites are omitted, as well as monomers, that are needed to complete the straight lines. The elements in these subfigure are the building blocks needed to form all possible graphs.

Also if we include the minus sign in the action, the contribution is $+1$, as the we have $(-1)^2$. Since all GV's at site i are involved, no other GV-pair can occur at site i , if there are already the two monomer pairs. Alternatively, the product of the GV's of corner a) and b) or the GV's of corner c) and d) provide all GV's for site i as well. That yields

$$a) \cdot b) = h_{x_i}^x v_{x_i}^o v_{x_i}^x h_{x_i}^o = -h_{x_i}^x h_{x_i}^o v_{x_i}^x v_{x_i}^o$$

and the integral gives -1 . or

$$c) \cdot d) = v_{x_i}^x h_{x_i}^x v_{x_i}^o h_{x_i}^o = -h_{x_i}^x h_{x_i}^o v_{x_i}^x v_{x_i}^o,$$

which also gives -1 after the integral. These 3 terms have to be added, as they all yield an empty site. So the total weight of an empty site is -1 . Next we consider the contribution of a closed loop. It is produced by a

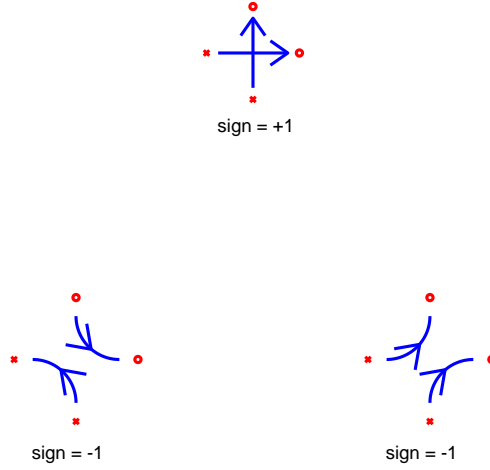


Figure 2.3: *There are three possible combinations of GV-pairs that represent empty sites. The weights add up to -1 .*

suitable product of GV-pairs

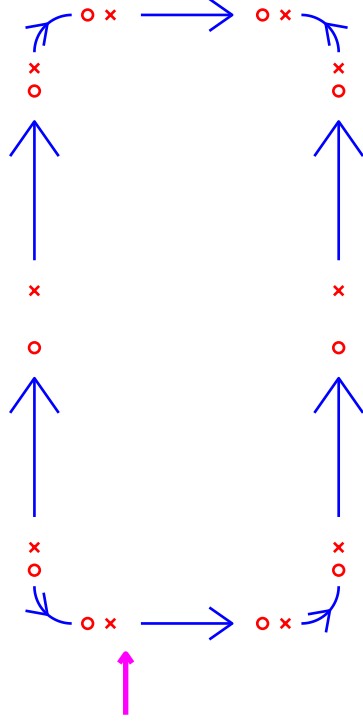
$$\prod_{n=1}^L P_n$$

each consisting of two GVs with a site and a type index.

We pick out one of the bond pair. It has site indices i_1 and i_2 and type indices α_1, α_2 . Then from the remaining set of GV-pairs we take the one that contains in one of the two variables the site index i_2 and the complement of α_2 , i.e. $\bar{\alpha}_2$. By the complement we mean the opposite flavor value but the same directional value, i.e. $(hx) \leftrightarrow (ho)$ and $(vx) \leftrightarrow (vo)$. The other variable shall have site index i_3 and type index α_3 . If the first operator in the second GV-pair is the one that matches the second variable of the first pair, then we have a factor $+1$ otherwise a factor -1 .

When we use the graphical representation of the GV-pairs, the first is an arrow with a x at its beginning and an o at its end. Now we attach the graphical element of the second GV-pair. The arrow already indicates whether or not the variables are in the required order. I.e. If we move opposite the arrow direction we get a minus sign. In addition, if the contracted pair of variables $\eta_{i_2}^{\alpha_2}$ and $\eta_{i_2}^{\bar{\alpha}_2}$ have the flavors ox that the trace gives $+1$ otherwise for xo we obtain -1 . Next, we seek again the pair that now contains site i_3 and type $\bar{\alpha}_3$. Again we obtain a factor -1 if we move opposite the arrow direction and another -1 if the flavor -sequence is xo . Now we move on like this. At the last step there is a final dangling (not contracted) variable with site index

that has to be equal to i_1 and a type index equal to $\bar{\alpha}_1$. Otherwise, the trace over these the GV-pairs vanishes and they do not form a admitted graph. By now we have reordered the GV pairs (which causes no sign). Again we obtain the two possible signs. Finally, we move the dangling variable to the front of the GV-pair product, which gives an additional minus sign. Finally, we analyze the sign of the so-produce flavor sequence at the first variable pair. The procedure is represented in figure 2.4. We begin the tour with an arrow

Figure 2.4: *Example.*

of a graph-line, here the point indicated by the magenta arrow. Then we move to the right, the signs from the arrow directions are: $+++++-----+$, i.e. the sign of the arrows is $(-1)^4 = +1$. Next we count how often we have the flavor -sequence xo , when we move in the direction of the first arrow. There are 5 such events. Hence the sign factor is $(-1)^5 = -1$. The two sign contributions give -1 , together with the additional -1 from moving the last variable to the front. The trace of the product of GV-pairs is $+1$. Keep in mind, that GV-pairs commute.

Basic elements of directed graphs

In order to determine the weight of connected graph elements it is necessary to take the direction into account, in which a graph is passed through. Therefore we have to consider directed graphs. Each graph has the 12 basic building blocks. There are 4 straight lines as shown in figure 2.5, that go tight, left, up, or down. The actual elements that form these lines are rep-

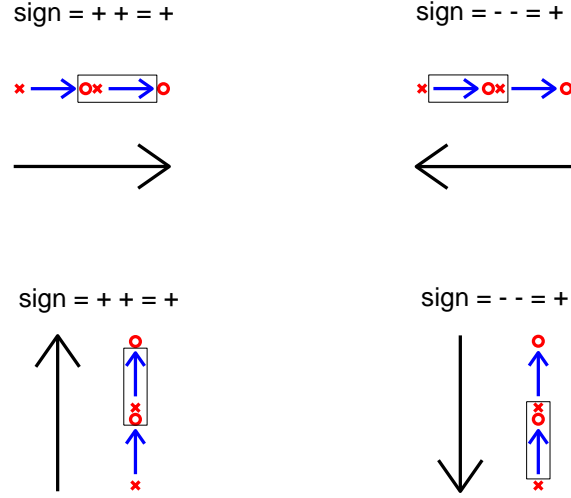


Figure 2.5: *The 4 different straight paths and their signs. We see that they all have a positive sign.*

resented in the black boxes. In all cases the sign of the order of the flavors ox and the arrow are the same, resulting in $+1$ for all lines. This is the sign that comes from the trace.

In addition to the lines there are 8 different corners as depicted in figure 2.7. With these elements we can construct any arbitrary graph and compute the

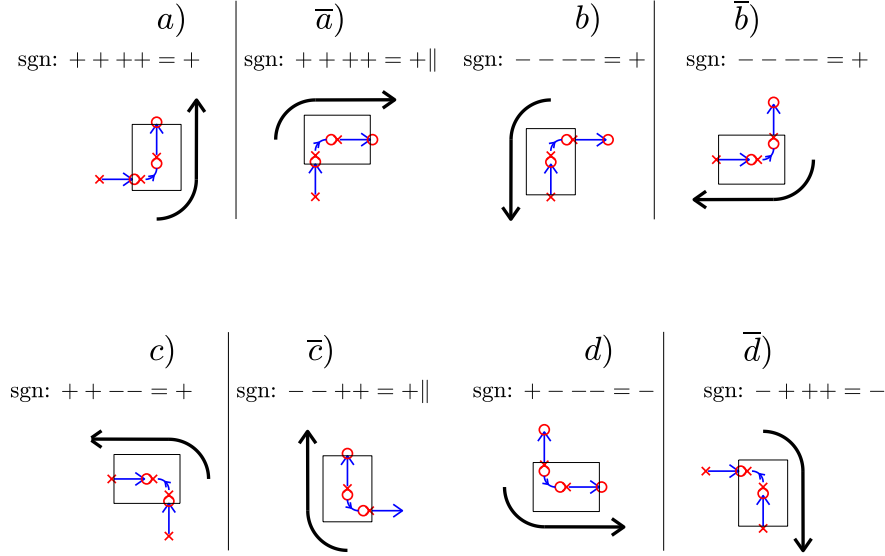


Figure 2.6: The 8 different paths around a corner and their signs. The notation is chosen such, that paths x and \bar{x} start at end at the same connecting points to the rest of the graph, but they are bend in opposite directions.

corresponding weigh/ sign. Let us reconsider the example given in figure 2.4. In the new elements of directed graphs it is We find the same sign as

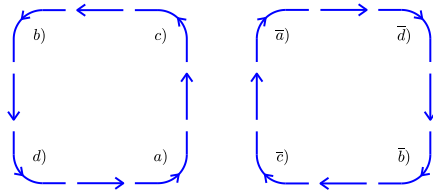


Figure 2.7: Example in directed graphs traversed in different directions.

before, namely $+1$: we have one minus sign from corner d or \bar{d} and one sign from closing the loop. Lets now consider a more complex example of closed non-overlapping loop:

We can start any closed non-crossing loop from the simple square, which has a positive sign, deform it. Each elementary deformation consists of $x - \bar{x}$ -

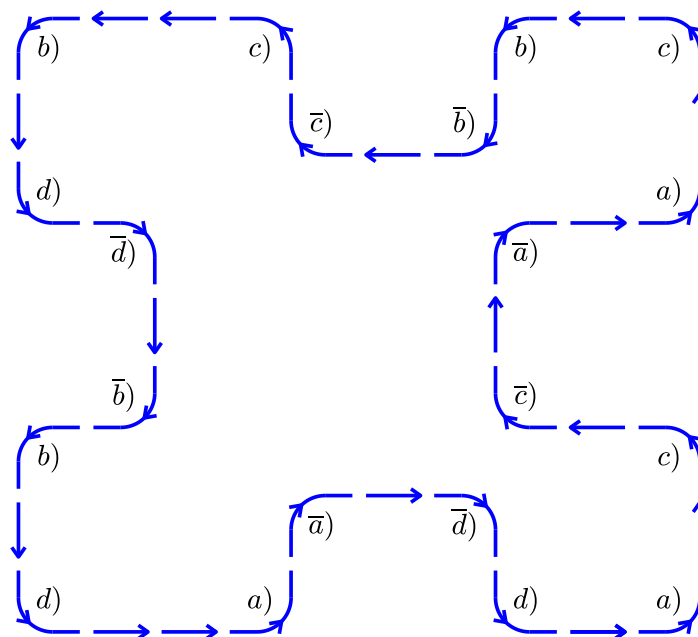


Figure 2.8: *More complex example for directed graphs.*

pairs, as can be seen in figure 2.8. But the sign of such pairs is always one. Hence, a closed loops has positive sign

Impact of the minus sign in the action terms

To each corner there is associated a minus sign from the action. And also each monomer required between lines passing straight through a site there is also a minus sign. Remember that the trace over the monomer variables of a sing GV-pair is one. I.e. at each site of a loop we have a minus. Empty sites also have a minus as discussed before. The signs of the action terms does not contribute, since always two terms enter and the sign squared is always on. We will see next that also a crossing will yield a minus sign. From the GV-elements we do not get a minus sign

Sign of crossings

We consider 2 closed loops, represented by the ellipses connected by a crossing. The overall sign is obtained by the signs of the elements in the ellipses, the sign of the crossing and the sign for closing this single connected graph. As before, also polygons with crossing are formed by a unique sequence of GV-pairs. And we obtain one extra sign from moving the dangling variable from the end to the beginning (closing sign). The direction of the path is uniquely given by the arrows. The directions how the crossing is passed through, specifies two isolated ellipses. In any case, the directions of the corners are always pairs of the form x and \bar{x} . The total sign of the two separated graph elements (GE) consists of the sign from the elements of the the two GE, The sign of the $x\text{-}\bar{x}$ pair and two closing sign. Corner pairs x / \bar{x} both have the same starting and end point and are bend in opposite directions. On the other hand we know the sign of the isolates objects already (proof by induction) as S_{l_i} . Then we have for the isolated loops

$$\begin{aligned} S_{e_1} * S_{e_2} * \underbrace{S_x * S_{\bar{x}}}_{=1} * \underbrace{S_{\text{closing}}^2}_{=1} &= S_{l_1} * S_{l_2} \\ \Rightarrow S_{e_1} * S_{e_2} &= S_{GE_1} * S_{GE_2} . \end{aligned}$$

and the overall sign of the connected graph, that has only one additional crossing is

$$S_{\text{total}} = S_{e_1} * S_{e_2} * \underbrace{S_{\text{str.lines}}}_{=1} * \underbrace{S_{\text{closing}}}_{=-1} = -S_{GE_1} * S_{GE_2} \quad (2.5)$$

Of course, the disconnected graph elements have to be shifted apart to obtain an admissible graph, but that has no impact on the sign argument.

Let's begin with a situation, where the separated graph elements are simple loops. Then both have a positive sign. The resulting connected graph with one crossing then has a negative sign.

We pick out any connected graph elements with $N_c \geq 1$ and separate it at one of the crossings, such that one of the resulting separate objects is a loop with zero crossings and the other has therefore $N_c - 1$ crossings. The sign of a graph element with N_c crossings is then according equation (2.5)

$$\begin{aligned} S_{N_c} &= (-1) * S_{N_c-1} * \underbrace{S_{N_c=0}}_{=1} = -S_{N_c-1} \\ \Rightarrow \quad S_{N_c} &= (-1)^{N_c} . \end{aligned}$$

Hence each crossing in a graph introduces a minus sign. The origin is the trace. From the building blocks there is no sign, as they are made of 4 bond GV-pairs, i.e. they add a factor t^4 , which is accounted for explicitly.

So we have the following situation: An empty site obtains a minus sign and a site obtaining GV-pairs that from a crossing also have a minus sign, which results in both cases from the trace. The signs in front of the GV-s in the actions is $+1$ as the GV-pairs occur in pairs in order to form an empty site or crossing. This is different at straight lines and corners. At sites, where straight lines pass through, a monomer is needed. Its contribution to the trace is $+1$, but it also has a weight factor a_m , which now enters individually and not in pairs as in the case of empty sites. Hence a site with a straight line passing through gets a factor a_m . A site with a corner gets in addition to its contribution to the trace a factor a_c .

Since crossings and empty sites contribute unavoidably a minus sign to the corresponding sites, it is necessary to choose $a_m = a_{corner} = -1$, to make all sites equal. Now they all contribute -1 . Hence, we have to correct the partition function by an overall factor

$$(-1)^N ,$$

which in case of an even number of sites vanishes.

2.1.2 Fourier transform of Grassmann variables

We introduce the Fourier transform $\eta_{\mathbf{k}}^\alpha$ of the GVs η_i^α :

$$\eta_{\mathbf{k}}^\alpha = \frac{1}{\sqrt{N}} \sum_i \eta_i^\alpha e^{i\mathbf{x}_i \mathbf{k}} \quad (2.6)$$

$$\eta_{\mathbf{x}_i}^\alpha = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}}^{1.b.z.} \eta_{\mathbf{k}}^\alpha e^{-i\mathbf{x}_i \mathbf{k}} , \quad (2.7)$$

and for the integral

$$d\eta_{\mathbf{k}}^\alpha = \frac{1}{\sqrt{N}} \sum_i d\eta_i^\alpha e^{-i\mathbf{x}_i \mathbf{k}} \quad (2.8)$$

$$d\eta_{\mathbf{x}_i}^\alpha = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}}^{1.b.z.} d\eta_{\mathbf{k}}^\alpha e^{i\mathbf{x}_i \mathbf{k}} . \quad (2.9)$$

The Fourier-transformed GVs are also GVs:

$$\eta_{\mathbf{k}}^\alpha \eta_{\mathbf{k}'}^{\alpha'} = -\eta_{\mathbf{k}'}^{\alpha'} \eta_{\mathbf{k}}^\alpha , \quad (2.10)$$

which is seen by inserting the definition and using the anti-commuting properties of the original GVs. The FT GVs also have the correct integral properties, that follow from

$$\int d\eta_{\mathbf{x}_i}^\alpha = 0 \quad (2.11a)$$

$$\int d\eta_{\mathbf{x}_i}^\alpha \eta_{\mathbf{x}_{i'}}^{\alpha'} = \delta_{\alpha\alpha'} \delta_{ii'} . \quad (2.11b)$$

Then

$$\int d\eta_{\mathbf{k}}^\alpha = 0$$

$$\int d\eta_{\mathbf{k}}^\alpha \eta_{\mathbf{k}'}^{\alpha'} = \delta_{\mathbf{k},\mathbf{k}'} \delta_{\alpha\alpha'} .$$

The proof of the first property is simply obtained by inserting the definition of the FT and using equation (2.11a) . The proof of the second equation is as follows

$$\begin{aligned} \int d\eta_{\mathbf{k}}^\alpha \eta_{\mathbf{k}'}^{\alpha'} &= \frac{1}{N} \sum_{i,j} e^{i(-\mathbf{k}\mathbf{x}_i + \mathbf{k}'\mathbf{x}_j)} \underbrace{\int d\eta_{\mathbf{x}_i}^\alpha \eta_{\mathbf{x}_j}^{\alpha'}}_{=\delta_{i,j}\delta_{\alpha,\alpha'}} \\ &= \frac{1}{N} \sum_i e^{i(-\mathbf{k}+\mathbf{k}')\mathbf{x}_i} = \delta_{\mathbf{k},\mathbf{k}'} \end{aligned}$$

After FT the action reads

$$A = A_{\text{bonds}} + A_{\text{corners}} + A_{\text{monomers}} \quad (2.12a)$$

$$A_{\text{bonds}} = \sum_{\mathbf{k}} (\varepsilon(k_x) h_{\mathbf{k}}^x h_{-\mathbf{k}}^o + \varepsilon(k_y) v_{\mathbf{k}}^x v_{-\mathbf{k}}^o) \quad (2.12b)$$

$$A_{\text{corners}} = - \sum_{\mathbf{k}} (h_{\mathbf{k}}^x v_{-\mathbf{k}}^o + v_{\mathbf{k}}^x h_{-\mathbf{k}}^o + v_{\mathbf{k}}^x h_{-\mathbf{k}}^x + v_{\mathbf{k}}^o h_{-\mathbf{k}}^o) \quad (2.12c)$$

$$A_{\text{monomers}} = \sum_{\mathbf{k}} (h_{\mathbf{k}}^x h_{-\mathbf{k}}^o + v_{\mathbf{k}}^x v_{-\mathbf{k}}^o) . \quad (2.12d)$$

We can combine the bonds and the monomers to

$$A_{\text{bpm}} = \sum_{\mathbf{k}} \left(\tilde{\varepsilon}(k_x) h_{\mathbf{k}}^x h_{-\mathbf{k}}^o + \tilde{\varepsilon}(k_y) v_{\mathbf{k}}^x v_{-\mathbf{k}}^o \right)$$

$$\tilde{\varepsilon}(k) = 1 + \varepsilon(k) = 1 + t e^{ik} .$$

In the sum we omit the term $\mathbf{k} = 0$, as it has a vanishing contribution in the thermodynamic limit. Next we use the ordering of the We can also use the GV-properties to symmetries the action by adding the term where the pair of GVs are swapped and $\mathbf{k} \rightarrow -\mathbf{k}$.

$$A = A_{\text{bpm}} + A_{\text{corners}}$$

$$A_{\text{bpm}} = \frac{1}{2} \sum_{\mathbf{k}} \left(\tilde{\varepsilon}(k_x) h_{\mathbf{k}}^x h_{-\mathbf{k}}^o - \tilde{\varepsilon}(-k_x) h_{\mathbf{k}}^o h_{-\mathbf{k}}^x + \tilde{\varepsilon}(k_y) v_{\mathbf{k}}^x v_{-\mathbf{k}}^o - \tilde{\varepsilon}(k_y) v_{\mathbf{k}}^o v_{-\mathbf{k}}^x \right)$$

$$A_{\text{corners}} = -\frac{1}{2} \sum_{\mathbf{k}} \left(h_{\mathbf{k}}^x v_{-\mathbf{k}}^o - v_{\mathbf{k}}^o h_{-\mathbf{k}}^x + v_{\mathbf{k}}^x h_{-\mathbf{k}}^o - h_{\mathbf{k}}^o v_{-\mathbf{k}}^x \right. \\ \left. \dots + v_{\mathbf{k}}^x h_{-\mathbf{k}}^x - h_{\mathbf{k}}^x v_{-\mathbf{k}}^x + v_{\mathbf{k}}^o h_{-\mathbf{k}}^o - h_{\mathbf{k}}^o v_{-\mathbf{k}}^o \right)$$

We combine all GVs that belong to the same \mathbf{k} into a vector.

$$\eta_{\mathbf{k}} = \left(h_{\mathbf{k}}^x, h_{\mathbf{k}}^o, v_{\mathbf{k}}^x, v_{\mathbf{k}}^o \right)^T$$

Then the action can be written as

$$A = \frac{1}{2} \sum_{\mathbf{k}} \eta_{\mathbf{k}}^T M_{\mathbf{k}} \eta_{-\mathbf{k}} = \sum'_{\mathbf{k}} \eta_{\mathbf{k}}^T M_{\mathbf{k}} \eta_{-\mathbf{k}} .$$

$$\text{with } M_{\mathbf{k}} = \begin{pmatrix} & h^x & h^o & v^x & v^o \\ \hline h^x | & 0 & \tilde{\varepsilon}(k_x) & 1 & -1 \\ h^o | & -\tilde{\varepsilon}(-k_x) & 0 & 1 & 1 \\ v^x | & -1 & -1 & 0 & \tilde{\varepsilon}(k_y) \\ v^o | & 1 & -1 & -\tilde{\varepsilon}(-k_y) & 0 \end{pmatrix}$$

Here M is an anti-Hermitian matrix. The symbol $\sum'_{\mathbf{k}}$ indicates that \mathbf{k} are only taken from the half plane $k_y > 0$ or $k_y = 0$, if $k_x > 0$. The second half of the wave vectors is then given uniquely by $-\mathbf{k}$. Moreover, the symbol \sum' also excludes $\mathbf{k} = 0$, which has no impact in the thermodynamic limit.

The Jakobi determinant of the transformation of the measure from real space to momentum space is $+1$, as outlined in appendix ??.

Then the vectors $\eta_{\mathbf{k}} \eta_{-\mathbf{k}}$ contain independent GVs. Therefore, the trace gives

$$\text{tr} \{ e^A \} = \prod'_{\mathbf{k}} \text{tr} \left\{ e^{\sum_{\mathbf{k}} \eta_{\mathbf{k}}^T M_{\mathbf{k}} \eta_{-\mathbf{k}}} \right\} = \prod'_{\mathbf{k}} \det (M_{\mathbf{k}}) .$$

The determinant of $M_{\mathbf{k}}$ yields

$$\det(M_{\mathbf{k}}) = (1 + t^2)^2 - 2t(1 - t^2)(\cos(k_x) + \cos(k_y)) ,$$

which has the symmetry $\det(M_{-\mathbf{k}}) = \det(M_{\mathbf{k}})$. So we can also include the second half plane in \mathbf{k} -space in the product and also the term $\mathbf{k} = 0$ as it has vanishing weight in the thermodynamic limit. Finally, we have

$$Z = 2^N \cosh^{2N}(j) \prod_{\mathbf{k}}^{1.B.z.} \left((1 + t^2)^2 - 2t(1 - t^2)(\cos(k_x) + \cos(k_y)) \right)^{\frac{1}{2}} , \quad (2.13)$$

which is the Onsager result.

2.2 Grassmann algebra

An n -dimensional Grassmann algebra is the algebra generated by a set of (Grassmann) variables $\{\eta_i\}_{i=1:n}$, satisfying

$$\{\eta_i, \eta_j\} = 0, \quad (2.14)$$

i.e. they anti-commute, which implies in particular that $a_i^2 = 0$. The algebra generated by these variables contains all expressions of the form

$$f(\eta) = f_0 + \sum_{i=1}^n f_i \eta_i + \sum_{i < j} f_{ij} \eta_i \eta_j + \sum_{i < j < k} f_{ijk} \eta_i \eta_j \eta_k + \dots + f_{1\dots n} \eta_1 \eta_2 \dots \eta_n ,$$

with $f_{\bullet} \in \mathbb{C}$. Obviously, the highest order term is

$$f_{1\dots n} \eta_1 \eta_2 \dots \eta_n .$$

since higher order terms would contain GVs in higher order which is zero. We now define a left derivative $\partial_i := \partial_{a_i}$. The derivative gives zero on a monomial which does not contain the variable a_i . If the monomial does contain a_i , it is moved to the left (with the appropriate sign due to the exchanges) and then suppressed. The operation is extended by linearity to any element of the algebra. A right derivative can be defined similarly. From this definition the following rules can be obtained

$$\begin{aligned} \{\partial_{a_i}, a_j\} &= \delta_{ij} \\ \{\partial_{a_i}, \partial_{a_j}\} &= 0 . \end{aligned}$$

Integrals are defined as linear operations over the functions f with the property that they can be identified with the (left) derivatives. Correspondingly,

$$\int da_i f(a) = \partial_{a_i} f(a) . \quad (2.15)$$

Hence,

$$\begin{aligned} \int da_i &= 0 \\ \int da_i a_j &= \delta_{ij} . \end{aligned}$$

We also introduce a second set of GVs $\{\psi\}_{i=1:n}$ with the additional property

$$\{\psi_i, \eta_j\} = 0 , \quad \forall i, j .$$

Next we compute exponentials of the form

$$\int \dots \int \mathcal{D}_{\eta\psi} e^{\psi^T A \eta} = \int \dots \int \mathcal{D}_{\eta\psi} e^{\frac{1}{2} \sum_{ij} \psi_i A_{ij} \eta_j} \quad (2.16)$$

$$= \int \dots \int \mathcal{D}_{\eta\psi} \prod_{i < j} e^{A_{ij} \eta_i \eta_j} \quad (2.17)$$

$$= \int \dots \int \mathcal{D}_{\eta\psi} \prod_{i < j} \underbrace{(1 + A_{ij} \eta_i \eta_j)}_{=B_{ij}} . \quad (2.18)$$

The Grassmann-measure is defined as

$$\mathcal{D}_{\eta\psi} := \prod_i d\eta_i d\psi_i .$$

Hence

$$\int \dots \int \mathcal{D}_{\eta\psi} \prod_i \psi_i \eta_i = 1 . \quad (2.19)$$

We continue with equation (2.16) The double product can be formally written as

$$\prod_{ij} B_{ij} = \left[B_{11} \dots B_{1n} \right] \times \left[B_{21} \dots B_{2n} \right] \times \dots \times \left[B_{n1} \dots B_{nn} \right] \quad (2.20)$$

There are 2^{n^2} possible terms, by choosing the 1 or the term $A_{ij} \psi_i \eta_j$ from each B_{ij} -term. However, most of these combinations result in a vanishing trace

because some of the GVs occur several times or not at all. The only choices that give a non vanishing contribution to the trace are as follows: From each square bracket in equation (2.20) choose one and only one $A_{ij}\psi_i\eta_j$ and the other terms contribute 1. The contribution of the l -th square brackets is $A_{l,j_l}\psi_l\eta_{j_l}$. Thus, each ψ_i occurs precisely once. To ensure that this is also true for the η_j , the set of indices $\{j_l\}$ can only be permutations of the indices $\{1, 2, \dots, n\}$, which leads to

$$\int \dots \int \mathcal{D}_{\eta\psi} e^{\psi^T A \eta} = \sum_{\mathcal{P}} \left(\prod_{l=1}^n A_{l,\mathcal{P}_l} \right) \int \dots \int \mathcal{D}_{\eta\psi} \left(\prod_{l=1}^n \psi_l \eta_{\mathcal{P}_l} \right). \quad (2.21)$$

Finally, we need to bring the permuted indices back into the natural order. To this end, we first move the η_j GVs to the very end, by retaining there mutual order, i.e.

$$\prod_l \psi_l \eta_{\mathcal{P}_l} = \text{sign} \cdot \prod_l \psi_l \prod_l \eta_{\mathcal{P}_l}$$

Here, sign is the sign associated with separating the η - from the ψ -variables. Next we bring the η -s into their natural order

$$\prod_l \psi_l \eta_{\mathcal{P}_l} = \text{sign}(\mathcal{P}) \cdot \text{sign} \cdot \prod_l \psi_l \prod_l \eta_l$$

Eventually, we form again the $\eta - \psi$ -pairs, which again introduces the same sign as in the first step:

$$\begin{aligned} \prod_l \psi_l \eta_{\mathcal{P}_l} &= \text{sign}(\mathcal{P}) (\text{sign})^2 \prod_l \psi_l \eta_l \\ &= \text{sign}(\mathcal{P}) \prod_l \psi_l \eta_l \end{aligned}$$

Along with equation (2.19) [\[previous page\]](#) and equation (2.21), we have

$$\int \dots \int \mathcal{D}_{\eta\psi} e^{\psi^T A \eta} = \sum_{\mathcal{P}} \text{sign}(\mathcal{P}) \left(\prod_{l=1}^n A_{l,\mathcal{P}_l} \right).$$

and finally

GAUSSIAN INTEGRAL (of type I)
$\int \dots \int \mathcal{D}_{\eta\psi} e^{\psi^T A \eta} = \det(A). \quad (2.22)$

Gaussian integral II

In this section we compute exponentials of the form

$$\int \dots \int \mathcal{D}_\eta e^{\frac{1}{2} \eta^T A \eta} = \int \dots \int \mathcal{D}_\eta e^{\frac{1}{2} \sum_{ij} \eta_i A_{ij} \eta_j} . \quad (2.23)$$

The Grassmann-measure is defined now as

$$\mathcal{D}_\eta := d\eta_n d\eta_{n-1} \dots d\eta_1 .$$

In this case A has to be anti-Hermitian/ skew-symmetric , i.e.

$$\begin{aligned} A_{ji} &= -A_{ij} \\ \text{then } \frac{1}{2} \sum_{ij} \eta_i A_{ij} \eta_j &= \sum_{i < j} \eta_i A_{ij} \eta_j . \end{aligned}$$

We consider only the case of even dimension $n = 2m$. Then

$$\int \dots \int \mathcal{D}_\eta e^{\frac{1}{2} \eta^T A \eta} = \int \dots \int \mathcal{D}_\eta \prod_{i < j} e^{A_{ij} \eta_i \eta_j} \quad (2.24)$$

$$= \int \dots \int \mathcal{D}_\eta \prod_{i < j} \underbrace{(1 + A_{ij} \eta_i \eta_j)}_{= B_{ij}} \quad (2.25)$$

$$\prod_{i < j} B_{ij} = \left[B_{11} \dots B_{1n} \right] \times \left[B_{23} \dots B_{2n} \right] \times \dots \times \quad (2.26)$$

Each B_{ij} contributes either 1 or $\kappa_{ij} := A_{ij} \eta_i \eta_j$. The product splits into a sum of $2^{n \cdot n}$ terms $\{T_i\}_{i=1:n \cdot n}$. But a non-vanishing trace is only obtained if each GV occurs precisely once. This means that non vanishing terms T_i contain $(n/2 = m)$ κ_{ij} -terms, with no indices in common, or rather: each index from the list $\{1, 2, \dots, n\}$ occurs once. The κ_{ij} terms describe a pairing between indices i and j , with $i < j$. The non-vanishing combinations κ_{ij} terms therefore describes a partitioning of the set $\{1, 2, \dots, 2m\}$ into pairs, described by

$$\kappa_{i_1, j_1}, \kappa_{i_2, j_2}, \dots, \kappa_{i_m, j_m} .$$

Moreover, according to equation (2.26) , we have

$$\begin{aligned} i_l &< j_l \\ i_1 &< i_2 < i_3 \dots \\ j_1 &< j_2 < j_3 \dots \end{aligned}$$

Clearly, in the set of T_i -s all possible pairings occur once and only once. The set of all such pairings be denote by P . An element $\alpha \in P$ is characterised by

$$\alpha = \{(i_1^\alpha, j_1^\alpha), (i_2^\alpha, j_2^\alpha), \dots, (i_m^\alpha, j_m^\alpha)\}.$$

P has $(2m - 1)!!$ elements. According to the construction for the non-vanishing trace elements, we have $i_1^\alpha < i_2^\alpha < \dots < i_m^\alpha$ and $i_l^\alpha < j_l^\alpha$. The contribution of such a partitioning to the trace is

$$\prod_l A_{i_l^\alpha, j_l^\alpha} \cdot \int \dots \int \mathcal{D}_\eta \prod_l \eta_{i_l^\alpha} \eta_{j_l^\alpha},$$

Let $\mathcal{P}(\alpha)$ be the permutation required to transform the sequence $i_1^\alpha, j_1^\alpha, i_2^\alpha, j_2^\alpha, \dots, i_m^\alpha, j_m^\alpha$ into the natural sequence $1, 2, \dots, 2m$, then

$$\prod_l A_{i_l^\alpha, j_l^\alpha} \cdot \int \dots \int \mathcal{D}_\eta \prod_l \eta_{i_l^\alpha} \eta_{j_l^\alpha} = \text{sign}(\mathcal{P}(\alpha)) \cdot \prod_l A_{i_l^\alpha, j_l^\alpha} \cdot \underbrace{\int \dots \int \mathcal{D}_\eta \prod_i \eta_i}_{=1}.$$

Hence we have

$$\int \dots \int \mathcal{D}_\eta e^{\frac{1}{2} \eta^T A \eta} = \sum_{\alpha \in P} \text{sign}(\mathcal{P}(\alpha)) \prod_{l=1}^m A_{i_l^\alpha, j_l^\alpha} = \text{Pf}(A). \quad (2.27)$$

This is the definition of the Pfaffian. For $n = 2m$ the Pfaffian is related to the determinant via

$$(\text{Pf}(A))^2 = \det(A)$$

For the proof we use

$$A = U D U^T$$

$$D = \begin{pmatrix} 0 & \lambda_1 & \dots & & \\ -\lambda_1 & 0 & \dots & & \\ . & . & 0 & \lambda_2 & \dots \\ . & . & -\lambda_2 & 0 & \dots \end{pmatrix}$$

where U is unitary. We use also

$$\eta = U \xi, \quad (2.28)$$

and obtain

$$\begin{aligned} \frac{1}{2} \eta^T A \eta &= \frac{1}{2} \xi^T D \xi \\ &= \sum_{\nu=1}^m \lambda_\nu \xi_{2\nu-1} \xi_{2\nu} \end{aligned}$$

Then

$$\begin{aligned}
\int \dots \int \mathcal{D}_\eta e^{\frac{1}{2}\eta^T A \eta} &= \det(U) \int \dots \int \mathcal{D}_\xi \prod_{\nu=1}^m e^{\lambda_\nu \xi_{2\nu-1} \xi_{2\nu}} \\
&= \det(U) \prod_{\nu=1}^m \int \int d\xi_{2\nu} d\xi_{2\nu-1} e^{\lambda_\nu \xi_{2\nu-1} \xi_{2\nu}} \\
&= \det(U) \prod_{\nu=1}^m \underbrace{\int \int d\xi_{2\nu} d\xi_{2\nu-1} (1 + \lambda_\nu \xi_{2\nu-1} \xi_{2\nu})}_{=\lambda_\nu} \\
&= \det(U) \prod_{\nu=1}^m \lambda_\nu .
\end{aligned}$$

Next we compute the determinant of A

$$\begin{aligned}
\det(A) &= \det(UDU^T) = \underbrace{(\det(U))^2}_{=1} \det(D) \\
&= \det \begin{pmatrix} 0 & \lambda_1 & \dots & & \\ -\lambda_1 & 0 & \dots & & \\ \cdot & \cdot & 0 & \lambda_2 & \dots \\ \cdot & \cdot & -\lambda_2 & 0 & \dots \end{pmatrix} \\
&= \prod_{\nu=1}^m \det \begin{pmatrix} 0 & \lambda_\nu \\ -\lambda_\nu & 0 \end{pmatrix} \\
&= \prod_{\nu=1}^m \lambda_\nu^2 \\
&= \left(\prod_{\nu=1}^m \lambda_\nu \right)^2 \\
&= \text{Pf}(A)
\end{aligned}$$

Linear transformations

We perform a linear transformation on a set of n GVs $\{\eta\}_{i=1:n}$

$$\eta_i = A_{ij} \xi_j; . \quad (2.29)$$

The anti commutator is

$$\{\eta_i, \eta_{i'}\} = A_{ij} A_{i'j'} \underbrace{\{\xi_j, \xi_{j'}\}}_{=0} = 0 .$$

For the differential we need

$$\partial_{\eta_i} \eta_{i'} = \delta_{ii'}$$

We expect that the differential ∂_{η_i} will also be a linear function

$$\partial_{\eta_i} t a = B_{ij} \partial_{\xi_j}$$

with the above constraint leading to

$$\begin{aligned} B_{ij} A_{i'j'} \underbrace{\partial_{\eta_j} \eta_{j'}}_{=\delta_{jj'}} &= \delta_{ii'} \\ (BA^T)_{ii'} &= \delta_{ii'} \\ BA^T &= \mathbb{1} . \end{aligned}$$

So we have

$$B = (A^{-1})^T . \quad (2.30)$$

Especially for unitary transformations ($A^{-1} = A^\dagger$) we have

$$B = (A^\dagger)^T = A^* .$$

We are interested in these transformations in integrals

$$\int \dots \int \mathcal{D}_\eta f(\eta) .$$

Then

$$\begin{aligned} \mathcal{D}_\eta &= d\eta_n d\eta_{n-1} \dots d\eta_1 \\ &= -d\eta_1 d\eta_2 \dots d\eta_n \\ &= - \sum_{\{l_j\}} \left(\prod_{j=1}^n B_{jl_j} \right) d\xi_{l_1} d\xi_{l_2} \dots d\xi_{l_n} \end{aligned}$$

On the rhs each GV has to occur precisely once, otherwise there would be GVs that occur several times resulting in a vanishing contribution. Hence the sum over all indices is restricted to a sum over all permutations (\mathcal{P}) of the indices $1, \dots, n$

$$\begin{aligned} \mathcal{D}_\eta &= - \sum_{\mathcal{P}} \left(\prod_{j=1}^n B_{jP_j} \right) d\xi_{P_1} d\xi_{P_2} \dots d\xi_{P_n} \\ &= - \underbrace{\sum_{\mathcal{P}} \text{sign}(\mathcal{P}) \left(\prod_{j=1}^n B_{jP_j} \right)}_{=\det(B)} d\xi_1 d\xi_2 \dots d\xi_n \\ &= \det(B) d\xi_n d\xi_{n-1} \dots d\xi_1 \end{aligned}$$

Hence the final result reads

$$\mathcal{D}_\eta = \det(B) \mathcal{D}_\xi \quad (2.31)$$

Or rather along with equation (2.30) [\[previous page\]](#)

$$\int \dots \int \mathcal{D}_\eta f(\eta) = \det(A)^{-1} \int \dots \int \mathcal{D}_\xi \tilde{f}(\xi) \quad (2.32)$$

$$\tilde{f}(\xi) = f(A\eta) . \quad (2.33)$$

Fourier transformations

Especially for the Fourier transformation we have

$$\eta_j = \frac{1}{\sqrt{N}} \sum_l e^{i\mathbf{x}_j \mathbf{k}_l} \xi_l$$

$$A_{jl} = \frac{1}{\sqrt{N}} e^{i\mathbf{x}_j \mathbf{k}_l} .$$

In the Ising application we have 4 different GVs at each site and we generalize the FT accordingly

$$\eta_j^\alpha = \frac{1}{\sqrt{N}} \sum_l e^{i\mathbf{x}_j \mathbf{k}_l} \xi_l^\alpha \quad (2.34)$$

$$(2.35)$$

The measure was defined in equation (2.1) [\[p. 47\]](#). Here each variable h^x, h^o, v^x, v^o introduces a factor $\det(A)$. Since the Fourier transform is unitary, the determinant is $+/-$ and $\det^4(A) = 1$. We choose the order of \mathbf{k} -vectors as

$$(\mathbf{0}), (\mathbf{k}_1, -\mathbf{k}_1), (\mathbf{k}_2, -\mathbf{k}_2), \dots, (\mathbf{k}_{N/2}, -\mathbf{k}_{N/2}) ,$$

where the set \mathbf{k}_i is chosen such that

$$k_{i,x} \leq k_{i,y} .$$

2.3 Correlation functions

We compute the correlation for an even number $2k$ of GVs. For odd the correlation is zero. Proof: Let's start with one GV

$$\begin{aligned} \langle \eta_i \rangle &= \det(U) \sum_l U_{i,l} \langle \xi_l \rangle \\ &= \det(U) \sum_l U_{i,l} \int \dots \int \mathcal{D}_\xi \xi_l \prod_{\nu=1}^m \left(1 + \lambda_\nu \xi_{2\nu-1} \xi_{2\nu} \right) \end{aligned}$$

If $l = 2\mu$

$$\langle \eta_{i_1}, \eta_{i_2}, \dots, \eta_{i_{2k}} \rangle = \frac{1}{Z} \int \dots \int \mathcal{D}_\eta e^{\frac{1}{2} \eta^A \eta} \eta_{i_1}, \eta_{i_2}, \dots, \eta_{i_{2k}}$$

We use the transformation in equation (2.28) [p. 65] and obtain

$$\langle \eta_{i_1}, \eta_{i_2}, \dots, \eta_{i_{2k}} \rangle = \frac{1}{Z} \det(U) \sum_{\{l_i\}} \prod_{i=1}^{2k} U_{i_i, l_i} \int \dots \int \mathcal{D}_\eta \prod_{\nu=1}^m e^{\lambda_\nu \xi_{2\nu-1} \xi_{2\nu}} \xi_{l_1}, \xi_{l_2}, \dots, \xi_{l_{2k}}$$

Now a factor

$$e^{\lambda_\nu \xi_{2\nu-1} \xi_{2\nu}} = \left(1 + \lambda_\nu \xi_{2\nu-1} \xi_{2\nu} \right)$$

ensures that from the pair of GVs $\xi_{2\nu-1} \xi_{2\nu}$ either both variables occur (a) in the correlation factors or none (b). In case (b) the integral gives λ_ν and in case (a) the integral ± 1 . The sign depends on the position of the two GVs in the correlation-sequence. We recall that the partition function yield

$$Z = \prod_{\nu=1}^m \lambda_\nu .$$

The division by Z therefore eliminates all factors λ_ν from the integrals of type b and integrals of type (a) are replaced by $\pm \lambda_\nu^{-1}$.

Hence, first we need all complete (ordered, otherwise we would count twice) pairings P of $2k$ elements and secondly we have to assign to each pair one of the possible index-pairs

$$(2\nu - 1, 2\nu) ,$$

or rather the index ν . Actually, none of the ν -indices should occur twice. On the other hand, if they occur repeatedly, the integral is zero anyways. Hence we allow the pairs to have all indices $\nu = 1, \dots, m$. The sum over $\{l_i\}$ is replaced by the sum over all elements α of complete (ordered) pairings, here represented by $\{(i_1^\alpha, i_2^\alpha), (i_3^\alpha, i_4^\alpha), \dots, (i_{2k-1}^\alpha, i_{2k}^\alpha)\}$, and all permutations \mathcal{P} of these $2k$ indices. Hence l_j are replaced by $i_{\mathcal{P}_j}^\alpha$. Then we have

$$\langle \eta_{i_1}, \eta_{i_2}, \dots, \eta_{i_{2k}} \rangle = \frac{1}{Z} \det(U) \prod_{i=1}^{2k} U_{i_i, l_i} \int \dots \int \mathcal{D}_\eta \prod_{\nu=1}^m e^{\lambda_\nu \xi_{2\nu-1} \xi_{2\nu}} \xi_{l_1}, \xi_{l_2}, \dots, \xi_{l_{2k}}$$

First we identify the pairing $\alpha \in P$ according to $\alpha = \{(I_1^\alpha, J_1^\alpha), (I_2^\alpha, J_2^\alpha), \dots, (I_k^\alpha, J_k^\alpha)\}$ and group the terms accordingly

$$\begin{aligned} \langle \eta_{i_1}, \eta_{i_2}, \dots, \eta_{i_{2k}} \rangle &= \frac{1}{Z} \det(U) \sum_{\{l_i\}} \int \dots \int \mathcal{D}_\eta \prod_{\nu=1}^m e^{\lambda_\nu \xi_{2\nu-1} \xi_{2\nu}} \prod_{\nu=1}^k U_{i_{I_\nu^\alpha}, l_{I_\nu^\alpha}} U_{i_{J_\nu^\alpha}, l_{J_\nu^\alpha}} \text{sign}(p(\alpha)) \prod_{\nu=1}^k \xi_{l_{I_\nu^\alpha}} \\ &= \frac{1}{Z} \text{sign}(p(\alpha)) \det(U) \int \dots \int \mathcal{D}_\eta \prod_{\nu=1}^m e^{\lambda_\nu \xi_{2\nu-1} \xi_{2\nu}} \prod_{\nu=1}^k \left(\sum_{l_{I_\nu^\alpha}, l_{J_\nu^\alpha}} U_{i_{I_\nu^\alpha}, l_{I_\nu^\alpha}} U_{i_{J_\nu^\alpha}, l_{J_\nu^\alpha}} \xi_{l_{I_\nu^\alpha}} \right) \end{aligned}$$

The sign is necessary, since we have permuted the GVs such that pairs are nearest neighbours and also have increasing indices in agreement with the definition of ordered pairings. Now we can rename the summation indices

$$\begin{aligned} \langle \eta_{i_1}, \eta_{i_2}, \dots, \eta_{i_{2k}} \rangle &= \frac{1}{Z} \text{sign}(p(\alpha)) \det(U) \\ &\quad \dots \int \dots \int \mathcal{D}_\eta \prod_{\nu=1}^m e^{\lambda_\nu \xi_{2\nu-1} \xi_{2\nu}} \prod_{\nu=1}^k \left(\sum_{l_1, l_2} U_{i_{I_\nu^\alpha}, l_1} U_{i_{J_\nu^\alpha}, l_2} \xi_{l_1} \xi_{l_2} \right). \end{aligned}$$

The idea of the pairing was to identify two GVs that belong to an index-pair of the form $(2\nu - 1, 2\nu)$. Each pair should have a different index ν . On the other hand, it does not matter if several pairs have the same index as the contribution is zero.

So the indices (l_1, l_2) can run over all pairs of the form $(2\nu - 1, 2\nu)$, i.e.

$$\begin{aligned} \langle \eta_{i_1}, \eta_{i_2}, \dots, \eta_{i_{2k}} \rangle &= \frac{1}{Z} \text{sign}(p(\alpha)) \det(U) \\ &\quad \dots \int \dots \int \mathcal{D}_\eta \prod_{\nu=1}^m e^{\lambda_\nu \xi_{2\nu-1} \xi_{2\nu}} \prod_{\nu=1}^k \left(\sum_{\mu} U_{i_{I_\nu^\alpha}, 2\mu-1} U_{i_{J_\nu^\alpha}, 2\mu} \xi_{2\mu-1} \xi_{2\mu} \right). \end{aligned}$$

2.4 Correlations of type I

For the Grassmann-pdf

$$e^{\psi^T A \eta} = e^{\sum_{ij} \psi_i A_{ij} \eta_j}$$

we compute the correlation function

$$\langle \psi_{i_1} \eta_{j_1} \psi_{i_2} \eta_{j_2} \dots \psi_{i_m} \eta_{j_m} \rangle.$$

If the number of GVs of type ψ and η differ, the correlation is zero. First we introduce the index sets:

$$\begin{aligned} I &= \{i_1, i_2, \dots, i_m\} \\ J &= \{j_1, j_2, \dots, j_m\} \end{aligned}$$

Next, we reorder the GVs such that the GVs in the correlator come first and the remaining GVs remain the original relative order.

$$\begin{aligned}\{\psi_1, \psi_2, \dots, \psi_{j_m}\} &\longrightarrow \{\psi_{i_1}, \psi_{i_2}, \dots, \psi_{i_m}, \dots\} \\ \{\eta_1, \eta_2, \dots, \eta_{j_m}\} &\longrightarrow \{\eta_{j_1}, \eta_{j_2}, \dots, \eta_{j_m}, \dots\}\end{aligned}$$

These reorderings can be achieved by permutations \mathcal{P} for the the GVs ψ and \mathcal{P}' for the GVs η . These reorderings of GVs are associated with signs: $\sigma_I = \text{sign}(\mathcal{P})$ and $\sigma_J = \text{sign}(\mathcal{P}')$, respectively. As far as the measure $\mathcal{D}_{\eta\psi}$ is concerned, we first separate the η and ψ , resulting in some sign σ . Then we bring these terms into the new order, associated with the sign $\sigma_I \cdot \sigma_J$. Finally, we interleaf the η and ψ terms again. The last step compensates the first sign σ . The new measure shall be denoted by $\tilde{\mathcal{D}}_{\eta\psi}$, for which we have

$$\mathcal{D}_{\eta\psi} = \sigma_I \cdot \sigma_J \cdot \tilde{\mathcal{D}}_{\eta\psi}.$$

We continue with

$$\begin{aligned}\langle \psi_{j_1} \eta_{i_1} \psi_{j_2} \eta_{i_2} \dots \psi_{j_m} \eta_{i_m} \rangle &= \frac{\sigma_I \sigma_J}{\det(A)} \int \dots \int \tilde{\mathcal{D}}_{\eta\psi} e^{\psi^T A \eta} \psi_{i_1} \eta_{j_1} \psi_{i_2} \eta_{j_2} \dots \psi_{i_m} \eta_{j_m} \\ &= \frac{\sigma_I \sigma_J}{\det(A)} \int \dots \int \tilde{\mathcal{D}}_{\eta\psi} \prod_{ij} (1 + A_{ij} \psi_i \eta_j) \psi_{i_1} \eta_{j_1} \psi_{i_2} \eta_{j_2} \dots \psi_{i_m} \eta_{j_m}\end{aligned}$$

All terms $(1 + A_{ij} \psi_i \eta_j)$ with $i \in I$ or $j \in J$ can be replace by 1, because the term $A_{ij} \psi_i \eta_j$ is multiplied ψ_i or η_j , leading to GV². Then the integral over the GVs contained in the correlator terms can be performed and gives 1. Then we merely have to integrate over the remaining GVs

$$\langle \psi_{j_1} \eta_{i_1} \psi_{j_2} \eta_{i_2} \dots \psi_{j_m} \eta_{i_m} \rangle = \frac{\sigma_I \sigma_J}{\det(A)} \int \dots \int \mathcal{D}_{\eta\psi}^{\not{I}, \not{J}} \left(\prod_{i \notin I, j \notin J} (1 + A_{ij} \psi_i \eta_j) \right)$$

where $\mathcal{D}_{\eta\psi}^{\not{I}, \not{J}}$ is the original measure $\mathcal{D}_{\eta\psi}$ containing only the indices $i \notin I$ and $j \notin J$. The result is that of the partition function for the action matrix $A^{\not{I}, \not{J}}$. Hence

$$\langle \psi_{j_1} \eta_{i_1} \psi_{j_2} \eta_{i_2} \dots \psi_{j_m} \eta_{i_m} \rangle = \sigma_I \sigma_J \frac{\det(A^{\not{I}, \not{J}})}{\det(A)}$$

We recall that $A^{\not{I}, \not{J}}$ is the matrix that is obtained by deleting the indices I and J in the rows and columns of A . To proceed, we reorder the indices of the matrix as we did above for the GVs, such that the indices in I and J

come first. This is achieved by the permutation matrices (see section 2.7.4) $P^{\mathcal{P}}$ and $P^{\mathcal{P}'}$. We call the corresponding matrix \hat{A}

$$\hat{A} = (P^{\mathcal{P}})^T A P^{\mathcal{P}'} .$$

Then for the determinant we have

$$\begin{aligned} \det(\hat{A}) &= \det\left((P^{\mathcal{P}})^T A P^{\mathcal{P}'}\right) \\ &= \det(P^{\mathcal{P}}) \det(A) \det(P^{\mathcal{P}'}) . \end{aligned}$$

$$\det(A) = \det(\hat{A}) \sigma_I \sigma_J$$

We define the block-structure of \hat{A} as

$$\hat{A} = \begin{pmatrix} \hat{A}_{11} & \hat{A}_{12} \\ \hat{A}_{2,1} & \hat{A}_{22} \end{pmatrix} = \begin{pmatrix} A^{IJ} & A^{I\not{J}} \\ A^{\not{I}J} & A^{\not{I}\not{J}} \end{pmatrix} .$$

Where sub-block 11 contains $m \times m$ elements, namely those of the correlators. Then

$$\det(A^{\not{I}\not{J}}) = \det(\hat{A}_{22})$$

and therefore

$$\langle \psi_{j_1} \eta_{i_1} \psi_{j_2} \eta_{i_2} \dots \psi_{j_m} \eta_{i_m} \rangle = \frac{\det(\hat{A}_{22})}{\det(\hat{A})}$$

According to equation (2.69) [p. 87] we have

$$\langle \psi_{j_1} \eta_{i_1} \psi_{j_2} \eta_{i_2} \dots \psi_{j_m} \eta_{i_m} \rangle = \det\left((\hat{A}^{-1})_{11}\right)$$

and according to equation (2.66) [p. 85] we have

$$\hat{A}^{-1} = (P^{\mathcal{P}'})^T A^{-1} P^{\mathcal{P}}$$

and hence

$$\begin{aligned} \langle \psi_{j_1} \eta_{i_1} \psi_{j_2} \eta_{i_2} \dots \psi_{j_m} \eta_{i_m} \rangle &= \det\left(\left((P^{\mathcal{P}'})^T A^{-1} P^{\mathcal{P}}\right)_{11}\right) \\ &= \det\left(\left((A^{-1})_{JJ}\right)\right) . \end{aligned}$$

Here $(A^{-1})_{JI}$ is the sub matrix of the inverse of the original matrix A taken at the indices J and I . A special case is

$$\langle \psi_i \eta_j \rangle = \det \left((A^{-1})_{ji} \right) = (A^{-1})_{ji} .$$

Hence

$$\langle \psi_{i_1} \eta_{j_1} \psi_{i_2} \eta_{j_2} \cdots \psi_{i_m} \eta_{j_m} \rangle = \det \left(\langle \psi_I \eta_J \rangle \right) ,$$

which corresponds to the Wick expansion

$$\langle \psi_{i_1} \eta_{j_1} \psi_{i_2} \eta_{j_2} \cdots \psi_{i_m} \eta_{j_m} \rangle = \sum_{\mathcal{P}} \text{sgn} \{ \mathcal{P} \} \prod_{l=1}^m \langle \psi_{i_l} \eta_{j_{\mathcal{P}_l}} \rangle$$

2.5 Correlations of type II

For the Grassmann-pdf

$$e^{\frac{1}{2} \eta^T A \eta} = e^{\sum_{ij} \psi_i A_{ij} \eta_j}$$

where A is antisymmetric, we compute the correlation function

$$\langle \eta_{j_1} \eta_{i_2} \cdots \eta_{i_{2m}} \rangle .$$

If the number of GVs have to even, otherwise the correlation is zero. First we introduce the index sets:

$$I = \{i_1, i_2, \dots, i_{2m}\} .$$

Next, we reorder the GVs such that the GVs in the correlator come first and the remaining GVs remain the original relative order.

$$\{\eta_1, \eta_2, \dots, \eta_{2m}\} \longrightarrow \{\eta_{i_1}, \eta_{i_2}, \dots, \eta_{i_{2m}}, \dots\} .$$

These reorderings of GVs are associated with σ_I . As far as the measure \mathcal{D}_η is concerned, the reordering (here in reverse order) gives the same sign. The new measure shall be denoted by $\tilde{\mathcal{D}}_\eta$, and we have

$$\mathcal{D}_\eta = \sigma_I \tilde{\mathcal{D}}_\eta .$$

We continue with

$$\begin{aligned} \langle \eta_{i_1} \eta_{i_2} \cdots \eta_{i_{2m}} \rangle &= \frac{\sigma_I}{\text{Pf}(A)} \int \cdots \int \tilde{\mathcal{D}}_\eta e^{\frac{1}{2} \eta^T A \eta} \eta_{i_1} \eta_{i_2} \cdots \eta_{i_{2m}} \\ &= \frac{\sigma_I}{\text{Pf}(A)} \int \cdots \int \tilde{\mathcal{D}}_\eta \prod_{i < j} \left(1 + a_{ij} \eta_i \eta_j \right) \eta_{i_1} \eta_{i_2} \cdots \eta_{i_{2m}} . \end{aligned}$$

All terms $(1 + A_{ij}\eta_i\eta_j)$ with $i \in I$ or $j \in I$ can be replaced by 1, because the term $A_{ij}\eta_i\eta_j$ is multiplied by η_i or η_j , leading to GV^2 . Then the integral over the GVs contained in the correlator terms can be performed and it gives 1. After that we only have to integrate over the remaining GVs

$$\langle \eta_{i_1}\eta_{i_2}\dots\eta_{i_{2m}} \rangle = \frac{\sigma_I}{\text{Pf}(A)} \int \dots \int \mathcal{D}'_\eta \prod_{i \notin I < j \notin I} \left(1 + a_{ij}\eta_i\eta_j \right) \eta_{i_1}\eta_{i_2}\dots\eta_{i_{2m}} .$$

where \mathcal{D}'_η is the original measure \mathcal{D}_η containing only the indices $i \notin I$. The result is that of the partition function for the action matrix A'' . Hence

$$\langle \eta_{i_1}\eta_{i_2}\dots\eta_{i_{2m}} \rangle = \sigma_I \frac{\text{Pf}(A'')}{\text{Pf}(A)}$$

We recall that A'' is the matrix that is obtained by deleting the indices I in the rows and columns of A .

We introduce again the reordered matrix, here

$$\hat{A} = (P^P)^T A P^P ,$$

with the block structure

$$\hat{A} = \begin{pmatrix} \hat{A}_{11} & \hat{A}_{12} \\ \hat{A}_{21} & \hat{A}_{22} \end{pmatrix} = \begin{pmatrix} A^{I,I} & A^{I,I'} \\ A^{I',I} & A^{I',I'} \end{pmatrix}$$

We use again

$$\text{Pf}(\hat{A}) = \text{Pf}(P_I^T A P_I) = \det(P_I) \text{Pf}(A) = \sigma_I \text{Pf}(A) .$$

and

$$\text{Pf}(A'') = \text{Pf}(\hat{A}_{22}) ,$$

resulting in

$$\langle \eta_{i_1}\eta_{i_2}\dots\eta_{i_m} \rangle = \frac{\text{Pf}(\hat{A}_{22})}{\text{Pf}(\hat{A})}$$

With equation (2.63) [\[p. 84\]](#) we then have

$$\langle \eta_{i_1}\eta_{i_2}\dots\eta_{i_m} \rangle = \text{Pf}\left((- \hat{A}^{-1})_{11}\right) = \text{Pf}\left((- A^{-1})_{II}\right)$$

Especially for $I = i_1 i_2$ we obtain

$$\langle \eta_{i_1} \eta_{i_2} \rangle = \text{Pf} \left(- \begin{bmatrix} 0 & (A^{-1})_{i_1 i_2} \\ -(A^{-1})_{i_1 i_2} & 0 \end{bmatrix} \right) = -(A^{-1})_{i_1 i_2}$$

So $\langle \eta_{i_1} \eta_{i_2} \rangle$ are the matrix elements of $-A^{-1}$ and we finally have

$$\langle \eta_{i_1} \eta_{i_2} \dots \eta_{i_m} \rangle = \text{Pf}(M) \quad (2.36)$$

where the $2m \times 2m$ matrix M has the elements

$$M_{ll'} = \langle \eta_{i_l} \eta_{i_{l'}} \rangle \quad (2.37)$$

2.6 Correlations in the Ising model

For the spin-spin correlation we need correlations of the form

$$\left\langle \prod_{l=1}^m (a + b \psi_{i_l} \eta_{j_l}) \right\rangle = a^m \left\langle \prod_{l=1}^m (1 + c \psi_{i_l} \eta_{j_l}) \right\rangle$$

with $c = b/a$. The correlator term can also be written as

$$\begin{aligned} \prod_{l=1}^m (1 + c \psi_{i_l} \eta_{j_l}) &= e^{\sum_{ij} C_{ij} \psi_i \eta_j} \\ C_{ij} &= c \sum_{l=1}^m \delta_{i, i_l} \sum_{l=1}^m \delta_{j, j_l} \\ &= c \sum_l P_{il}^{\mathcal{P}} P_{jl}^{\mathcal{P}'} \\ C &= c P^{\mathcal{P}} (P^{\mathcal{P}'})^T \end{aligned}$$

The matrices $P^{\mathcal{P}}$ and $P^{\mathcal{P}'}$ have the size $N \times m$. Inserting yields

$$\left\langle \prod_{l=1}^m (1 + c \psi_{i_l} \eta_{j_l}) \right\rangle = \frac{1}{\det(A)} \int \dots \int \mathcal{D}_{\eta\psi} e^{\psi^T (A+C) \eta} \quad (2.38)$$

$$= \frac{\det(A+C)}{\det(A)} \quad (2.39)$$

$$= \frac{\det(A(\mathbb{1} + A^{-1}C))}{\det(A)} \quad (2.40)$$

$$= \frac{\det(A) \det(\mathbb{1} + A^{-1}C)}{\det(A)} \quad (2.41)$$

$$= \det(\mathbb{1} + A^{-1}C) . \quad (2.42)$$

The Taylor expansion gives

$$\begin{aligned} \ln(\det(\mathbb{1} + A^{-1}C)) &= \text{tr} \left\{ \ln(\mathbb{1} + A^{-1}C) \right\} \\ &= \sum_{\nu=1}^{\infty} C_{\nu} c^{\nu} \text{tr} \left\{ (A^{-1}P^{\mathcal{P}}(P^{\mathcal{P}'})^T)^{\nu} \right\} \end{aligned}$$

the trace terms are

$$\begin{aligned} \text{tr} \left\{ (A^{-1}P^{\mathcal{P}}(P^{\mathcal{P}'})^T)^{\nu} \right\} &= \text{tr} \left\{ A^{-1}(P^{\mathcal{P}})^T P^{\mathcal{P}'} \dots A^{-1}P^{\mathcal{P}}(P^{\mathcal{P}'})^T \right\} \\ &= \text{tr} \left\{ P^{\mathcal{P}'} A^{-1}(P^{\mathcal{P}})^T P^{\mathcal{P}'} \dots A^{-1}(P^{\mathcal{P}})^T \right\} \\ &= \text{tr} \left\{ \left((P^{\mathcal{P}'})^T A^{-1}P^{\mathcal{P}} \right)^{\nu} \right\} \end{aligned}$$

Hence

$$\det(\mathbb{1}_N + A^{-1}C) = \det(\mathbb{1}_m + c(P^{\mathcal{P}'})^T A^{-1}P^{\mathcal{P}})$$

$$\begin{aligned} \left((P^{\mathcal{P}})^T A^{-1}P^{\mathcal{P}'} \right)_{ll'} &= \sum_{ji} P_{j,l}^{\mathcal{P}'} (A^{-1})_{ij} P_{il'}^{\mathcal{P}} \\ &= (A^{-1})_{ji i_{l'}} \\ (P^{\mathcal{P}})^T A^{-1}P^{\mathcal{P}'} &= (A^{-1})_{JI} \end{aligned}$$

The correlation is therefore

$$\left\langle \prod_{l=1}^m (a + b\psi_{i_l}\eta_{j_l}) \right\rangle = a^m \left\langle \prod_{l=1}^m (1 + c\psi_{i_l}\eta_{j_l}) \right\rangle \quad (2.43)$$

$$= a^m \det((\mathbb{1} + cA^{-1})_{JI}) \quad (2.44)$$

$$= \det(M) \quad (2.45)$$

$$M = a\mathbb{1} + b(A^{-1})_{JI} . \quad (2.46)$$

For the simplest case we find

$$\langle a + b\psi_i\eta_j \rangle = a + b \langle \psi_i\eta_j \rangle \quad (2.47)$$

$$\Rightarrow (A^{-1})_{ji} = \langle \psi_i\eta_j \rangle . \quad (2.48)$$

The final result therefore reads

$$\left\langle \prod_{l=1}^m (a + b\psi_{i_l}\eta_{j_l}) \right\rangle = \det(M) \quad (2.49a)$$

$$M_{ij} = a\delta_{ij} + \langle \psi_{i_l}\eta_{j_j} \rangle , \quad i, j \in \{1, 2, \dots, m\} \quad (2.49b)$$

2.6.1 Transformation: spin correlation to GV correlation

We are interested in the spin-spin-correlation

$$C_m^x := \langle \sigma_{\mathbf{x}_0} \sigma_{\mathbf{x}_0 + m \mathbf{e}_x} \rangle .$$

Due to translational invariance, the result is independent of \mathbf{x}_0 . Since $\sigma_i^2 = 1$ we can replace the spin-spin-correlation function by

$$\begin{aligned} C_m^x &= \left\langle \prod_{j=0}^{m-1} \sigma_{\mathbf{x}_0 + j \mathbf{e}_x} \sigma_{\mathbf{x}_0 + (j+1) \mathbf{e}_x} \right\rangle \\ &= \left\langle \prod_{\langle ij \rangle \in L} \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} \right\rangle . \end{aligned}$$

where $\langle i, j \rangle$ are indices for nearest neighbour sites and L is the set of such indices corresponding to the sites of the form $(\mathbf{x}_0 + j \mathbf{e}_x, \mathbf{x}_0 + (j+1) \mathbf{e}_x)$, for $j = 0, \dots, m-1$. Then

$$C_m^x = \frac{ch^N(\beta t)}{Z} \sum_{\{\sigma_{\mathbf{x}_i}\}} \prod_{\langle ij \rangle} \left(1 + t \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} \right) \prod_{\langle ij \rangle \in L} \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} .$$

Next

$$\begin{aligned} \sum_{\{\sigma_{\mathbf{x}_i}\}} \prod_{\langle ij \rangle} \left(1 + t \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} \right) \prod_{\langle ij \rangle \in L} \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} &= \sum_{\{\sigma_{\mathbf{x}_i}\}} \prod_{\langle ij \rangle \notin L} \left(1 + t \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} \right) \prod_{\langle ij \rangle \in L} \left[\left(1 + t \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} \right) \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} \right] \\ &= \sum_{\{\sigma_{\mathbf{x}_i}\}} \prod_{\langle ij \rangle \notin L} \left(1 + t \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} \right) \prod_{\langle ij \rangle \in L} \left(\sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} + t \right) \\ &= \sum_{\{\sigma_{\mathbf{x}_i}\}} \prod_{\langle ij \rangle \notin L} \left(1 + t \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} \right) \prod_{\langle ij \rangle \in L} \left(1 + \frac{1}{t} \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} \right) \\ &= t^m \sum_{\{\sigma_{\mathbf{x}_i}\}} \prod_{\langle ij \rangle} \left(1 + \tilde{t}_{ij} \sigma_{\mathbf{x}_i} \sigma_{\mathbf{x}_j} \right) . \end{aligned}$$

with

$$\tilde{t}_{ij} = \begin{cases} t & \text{if } ij \notin L \\ t^{-1} & \text{if } ij \in L \end{cases}$$

This is (apart from the prefactor) the partition function of an Ising model with modified t . Then

$$C_m^x = t^m \frac{Z(\tilde{t})}{Z(t)} = \frac{\text{tr} \{e^{\tilde{A}}\}}{\text{tr} \{e^A\}}.$$

So it can be written as

$$\text{tr} \{e^{\tilde{A}}\} = \text{tr} \left\{ e^{A'} \prod_{ij}^{\in L} e^{t^{-1} h_{x_i}^x h_{x_j}^o} \right\}$$

Here A' is that part of the action, where the bonds on the nearest neighbour pairs in L are omitted.

$$\begin{aligned} t^m \text{tr} \{e^{\tilde{A}}\} &= t^m \text{tr} \left\{ e^{A'} \prod_{ij}^{\in L} e^{t h_{x_i}^x h_{x_j}^o} e^{-t h_{x_i}^x h_{x_j}^o} e^{t^{-1} h_{x_i}^x h_{x_j}^o} \right\} \\ &= t^m \text{tr} \left\{ e^A \prod_{ij}^{\in L} e^{(t^{-1} - t) h_{x_i}^x h_{x_j}^o} \right\} \\ &= t^m \text{tr} \left\{ e^A \prod_{ij}^{\in L} (1 + (t^{-1} - t) h_{x_i}^x h_{x_j}^o) \right\}. \end{aligned}$$

Hence

$$\begin{aligned} C_m^x &= \frac{t^m \text{tr} \{e^{\tilde{A}}\}}{\text{tr} \{e^A\}} \\ &= \frac{\text{tr} \left\{ e^A \prod_{ij}^{\in L} (t + (1 - t^2) h_{x_i}^x h_{x_j}^o) \right\}}{\text{tr} \{e^A\}} \\ &= \left\langle \prod_{ij}^{\in L} (t + (1 - t^2) h_{x_i}^x h_{x_j}^o) \right\rangle. \end{aligned}$$

In the present case for the spin-spin correlation in x-direction we have

$$C_m^x = \left\langle \prod_{i=0}^{m-1} (t + (1 - t^2) h_{(i,0)}^x h_{(i+1,0)}^o) \right\rangle.$$

When we compare with equation (2.49) [p. 76] the present case has $I =$

$\{(1, 0), (2, 0), \dots (m, 0)\}$ and $J = \{(2, 0), (3, 0), \dots (m + 1, 0)\}$. Hence

$$C_m^x = \det(M) \quad (2.50)$$

$$M_{ij} = t\delta_{ij} + (1 - t^2) \langle h_{I_i}^x h_{J_j}^o \rangle \quad (2.51)$$

$$= t\delta_{ij} + (1 - t^2) \langle h_i^x h_{j+1}^o \rangle \quad (2.52)$$

$$(2.53)$$

2.6.2 Computation of pair-correlations

We use translational invariance and the Fourier transformation defined in equation (2.6) [p. 58] and compute

$$\begin{aligned} \langle h_{x_i}^x h_{x_j}^o \rangle &= \frac{1}{N} \sum_l \langle h_{x_l+x_i}^x h_{x_l+x_j}^o \rangle \\ &= \frac{1}{N} \sum_l \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}(x_l+x_i)} \frac{1}{\sqrt{N}} \sum_{\mathbf{k}'} e^{-i\mathbf{k}'(x_l+x_j)} \langle h_{\mathbf{k}}^x h_{\mathbf{k}'}^o \rangle \\ &= \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} \underbrace{\left(\frac{1}{N} \sum_l e^{-i(\mathbf{k}+\mathbf{k}')x_l} \right)}_{=\delta_{\mathbf{k}', -\mathbf{k}}} e^{-i(\mathbf{k}x_i + \mathbf{k}'x_j)} \langle h_{\mathbf{k}}^x h_{\mathbf{k}'}^o \rangle \\ &= \frac{1}{N} \sum_{\mathbf{k}} e^{i(x_j-x_i)\mathbf{k}} \langle h_{\mathbf{k}}^x h_{-\mathbf{k}}^o \rangle . \end{aligned}$$

Then

$$\langle h_{(i,0)}^x h_{(j+1,0)}^o \rangle = \frac{1}{N} \sum_{\mathbf{k}} e^{i(j+1-i)k_x} \langle h_{\mathbf{k}}^x h_{-\mathbf{k}}^o \rangle .$$

and

$$\delta_{ij} = \frac{1}{N} \sum_{\mathbf{k}} e^{i(j-i)k_x} .$$

Therefore

$$M_{ij} = \frac{1}{N} \sum_{\mathbf{k}} e^{i(j-i)k_x} \left[t + (1 - t^2) e^{ik_x} \langle h_{\mathbf{k}}^x h_{-\mathbf{k}}^o \rangle \right]$$

For the $\langle h_{\mathbf{k}}^x h_{-\mathbf{k}}^o \rangle$ correlation we merely need to consider the subspace for this particular \mathbf{k} . The corresponding action matrix is

$$A_{\mathbf{k}} = \begin{pmatrix} & h^x & h^o & v^x & v^o \\ \hline h^x | & 0 & \tilde{\varepsilon}(k_x) & 1 & -1 \\ h^o | & -\tilde{\varepsilon}(-k_x) & 0 & 1 & 1 \\ v^x | & -1 & -1 & 0 & \tilde{\varepsilon}(k_y) \\ v^o | & 1 & -1 & -\tilde{\varepsilon}(-k_y) & 0 \end{pmatrix}$$

In this enumeration we need

$$\langle \psi_1 \eta_2 \rangle = (A^{-1})_{21}$$

We obtain with MATHEMATICA

$$\begin{aligned} (A_{\mathbf{k}}^{-1})_{21} &= \frac{C_{\mathbf{k}}}{\det(A_{\mathbf{k}})} \\ C_{\mathbf{k}} &= -(\tilde{\varepsilon}(k_y) + \tilde{\varepsilon}(-k_y)) + \tilde{\varepsilon}(-k_x)|\tilde{\varepsilon}(k_y)|^2 \\ \det(A_{\mathbf{k}}) &= (1 + t^2)^2 - 2t(1 - t^2)(\cos(k_x) + \cos(k_y)) . \end{aligned}$$

2.7 Pfaffian

2.7.1 Definition

Let Π be the set of all partitions $\{1, 2, \dots, 2n\}$ in pairs. Each element $\alpha \in \Pi$ can be uniquely identified as

$$\alpha = \{(i_1, j_1), (i_2, j_2) \dots, (i_n, j_n)\} ,$$

it being understood that $i_1 < i_2 < \dots < i_n$ and $i_k < j_k \forall k$. We define

$$\mathcal{P} = \begin{bmatrix} 1 & 2 & 3 & 4 & \dots & 2n-1 & 2n \\ i_1 & j_1 & i_2 & j_2 & \dots & i_n & j_n \end{bmatrix}$$

as the corresponding permutation and we define $\text{sgn}\{\alpha\} = \text{sgn}\{\mathcal{P}\}$.

For any antisymmetric (skew-symmetric, alternating, i.e. $A_{ji} = -A_{ij}$) $2n \times 2n$ matrix A the Pfaffian is defined as

$$\text{Pf}(A) = \sum_{\alpha \in \Pi} \text{sgn}\{\alpha\} a_{i_1^\alpha j_1^\alpha} a_{i_2^\alpha j_2^\alpha} \dots a_{i_n^\alpha j_n^\alpha} \quad (2.54)$$

$$\text{Pf}(A) = \sum_{\alpha \in \Pi} \text{sgn}\{\alpha\} \prod_{l=1}^n a_{i_l^\alpha j_l^\alpha} \quad (2.55)$$

For anti-symmetric matrices of odd dimension the Pfaffian is defined as zero.

2.7.2 Examples

$$\begin{aligned} \text{Pf} \left(\begin{bmatrix} 0 & a \\ -a & 0 \end{bmatrix} \right) &= a \\ \text{Pf} \left(\begin{bmatrix} 0 & \lambda_1 & 0 & 0 \\ -\lambda_1 & 0 & \omega_1 & 0 \\ 0 & -\omega_2 & 0 & \lambda_2 \\ 0 & 0 & -\lambda_2 & 0 \end{bmatrix} \right) &= a_{12}a_{34} - a_{13}a_{24} + a_{14}a_{23} \\ &= \lambda_1 \lambda_2 . \end{aligned}$$

2.7.3 Properties

For any anti-symmetric $2n \times 2n$ matrix A or A_l and an arbitrary $2n \times 2n$ matrix B holds

$$\text{Pf}(A)^2 = \det(A) \quad (2.56a)$$

$$\text{Pf}(BAB^T) = \det(B) \cdot \text{Pf}(A) \quad (2.56b)$$

$$\text{Pf}(\lambda A) = \lambda^2 \text{Pf}(A) \quad (2.56c)$$

$$\text{Pf}(A^T) = (-1)^n \text{Pf}(A) \quad (2.56d)$$

for block-diagonal matrices

$$A = \oplus_{l=1}^L A_l = \begin{pmatrix} A_1 & & \\ & \ddots & \\ & & A_L \end{pmatrix}$$

$$\text{holds } \text{Pf}(A) = \prod_{l=1}^L \text{Pf}(A_l) \quad (2.56e)$$

for an arbitrary $n \times n$ matrix M holds

$$\text{Pf}\left(\begin{pmatrix} 0 & M \\ -M & 0 \end{pmatrix}\right) = (-1)^{\frac{n(n-1)}{2}} \det(M) . \quad (2.56f)$$

Any anti-symmetric $2n \times 2n$ matrix A can be written as

$$A = UDU^T ,$$

where $U^T = U^{-1}$ with $\det(U) = 1$ (*$\det(U) = 1$ can always be achieved by adjusting the sign of λ_ν*) and

$$D = \oplus_{\nu=1}^n D_\nu$$

$$D_\nu = \begin{pmatrix} 0 & \lambda_\nu \\ -\lambda_\nu & 0 \end{pmatrix}$$

From that we can proof that

$$\begin{aligned} \text{Pf}(A) &= \text{Pf}(UDU^T) = \underbrace{\det(U)}_{=1} \text{Pf}(D) = \prod_{\nu=1}^n \text{Pf}(D_\nu) \\ &= \prod_{\nu=1}^n \lambda_\nu . \end{aligned}$$

and

$$\begin{aligned}
\text{Pf}(A^{-1}) &= \text{Pf}(UD^{-1}U^T) = \det(U)\text{Pf}(D^{-1}) \\
&= \text{Pf}\left(\oplus_{\nu=1}^n (D_\nu)^{-1}\right) \\
&= \prod_{\nu=1}^n \text{Pf}\left((D_\nu)^{-1}\right) \\
&= \prod_{\nu=1}^n \text{Pf}\left(\begin{bmatrix} 0 & -1/\lambda_\nu \\ 1/\lambda_\nu & 0 \end{bmatrix}\right) \\
&= \prod_{\nu=1}^n \left(-\frac{1}{\lambda_\nu}\right) \\
&= (-1)^n \left(\text{Pf}(A)\right)^{-1}.
\end{aligned}$$

Or rather

$$\text{Pf}(A^{-1}) = \left(\text{Pf}(-A)\right)^{-1}. \quad (2.57)$$

We also easily find

$$\begin{aligned}
\det(A) &= \det(U) \det(D) \det(U^{-1}) = \det(\oplus_{\nu=1}^n D_\nu) \\
&= \prod_{\nu=1}^n \det(D_\nu) \\
&= \prod_{\nu=1}^n (\lambda_\nu)^2 \\
&= \left(\prod_{\nu=1}^n \lambda_\nu\right)^2.
\end{aligned}$$

Which proofs

$$\det(A) = \left(\text{Pf}(A)\right)^2 \quad (2.58)$$

Similar to the determinant we can use the block diagonalization of the anti-symmetric block-matrix

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

$$A = \begin{pmatrix} \mathbb{1} & -G \\ 0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} \tilde{A}_{11} & 0 \\ 0 & \hat{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ -F & \mathbb{1} \end{pmatrix} \quad (2.59)$$

With

$$\begin{aligned} F &= -(A_{22})^{-1} A_{21} \\ G &= -A_{12} (A_{22})^{-1} \end{aligned}$$

Due to the antisymmetry we have

$$\begin{aligned} A_{21} &= -A_{12}^T \\ A_{22}^T &= -A_{22} \end{aligned}$$

and therefore

$$\begin{aligned} F^T &= - \underbrace{A_{21}^T}_{=-A_{12}} \underbrace{\left((A_{22})^{-1} \right)^T}_{=-\left(A_{22} \right)^{-1}} \\ &= -A_{12} \left((A_{22})^{-1} \right)^T \\ &= -A_{12} (A_{22})^{-1} . \end{aligned}$$

I.e.

$$G = F^T \quad (2.60)$$

Moreover,

$$\begin{aligned} (\tilde{A}_{11})^T &= \left(A_{11} - A_{12} A_{22}^{-1} A_{21} \right)^T \\ &= \underbrace{A_{11}^T}_{=-A_{11}} - \underbrace{A_{21}^T}_{=-A_{12}} \underbrace{\left(A_{22}^{-1} \right)^T}_{=-A_{22}^{-1}} \underbrace{A_{12}^T}_{=-A_{21}} \\ &= - \left(A_{11} - A_{12} A_{22}^{-1} A_{21} \right) \\ &= -\tilde{A}_{11} . \end{aligned}$$

With

$$\mathcal{F} \quad (2.61)$$

$$\mathcal{F} := \begin{pmatrix} \mathbb{1} & 0 \\ -F & \mathbb{1} \end{pmatrix} \quad (2.62)$$

equation (2.59) leads to

$$A = \mathcal{F}^T \begin{pmatrix} \tilde{A}_{11} & 0 \\ 0 & \hat{A}_{22} \end{pmatrix} \mathcal{F}$$

Then

$$\begin{aligned} \text{Pf}(A) &= \underbrace{\det(\mathcal{F})}_{=1} \text{Pf} \left(\begin{bmatrix} \tilde{A}_{11} & 0 \\ 0 & \hat{A}_{22} \end{bmatrix} \right) \\ &= \text{Pf}(\tilde{A}_{11}) \text{Pf}(A_{22}) \end{aligned}$$

And as before

$$\tilde{A}_{11} = \left((A^{-1})_{11} \right)^{-1}.$$

So we have

$$\begin{aligned} \text{Pf}(\tilde{A}_{11}) &= \text{Pf} \left(\left((A^{-1})_{11} \right)^{-1} \right) \\ &= \left[\text{Pf}(-(A^{-1})_{11}) \right]^{-1}. \end{aligned}$$

Hence

$$\frac{\text{Pf}(A_{22})}{\text{Pf}(A)} = \text{Pf}(-(A^{-1})_{11}) = \text{Pf}((-A^{-1})_{11}) \quad (2.63)$$

2.7.4 Properties of permutation matrices

Let the permutation \mathcal{P} be defined by the mapping $i \rightarrow \mathcal{P}_i$, then we define the corresponding matrix as

$$P_{ij}^{\mathcal{P}} = \delta_{i, \mathcal{P}_j}. \quad (2.64)$$

It has the property

$$\det(P^{\mathcal{P}}) = \text{sgn}\{\mathcal{P}\}. \quad (2.65)$$

Proof

$$\begin{aligned}
\det(P^{\mathcal{P}}) &= \det\left((P^{\mathcal{P}})^T\right) \\
&= \sum_{\mathcal{P}'} \text{sgn}\{\mathcal{P}'\} \prod_i \left((P^{\mathcal{P}})^T\right)_{i, \mathcal{P}'_i} \\
&= \sum_{\mathcal{P}'} \text{sgn}\{\mathcal{P}'\} \prod_i P^{\mathcal{P}}_{\mathcal{P}'_i, i} \\
&= \sum_{\mathcal{P}'} \text{sgn}\{\mathcal{P}'\} \prod_i \underbrace{\delta_{\mathcal{P}'_i, \mathcal{P}_i}}_{=\delta_{\mathcal{P}, \mathcal{P}'}} \\
&= \text{sgn}\{\mathcal{P}'\}
\end{aligned}$$

q.e.d. ✓

We easily see that the permutation matrix is a unitary matrix, i.e. $P^T = P^{-1}$:

$$(P^T P)_{ij} = P_{li} P_{lj} = \sum_l \delta_{l, P_i} \delta_{l, P_j} = \delta_{P_i, P_j} = \delta_{ij} .$$

Moreover, the transformed matrix \hat{A} , where column and rows are permuted individually, is obtained by

$$\hat{A} = (P^{\mathcal{P}})^T A P^{\mathcal{P}'}$$

and has the matrix elements

$$\hat{A}_{ij} = P^{\mathcal{P}}_{li} A_{ll'} P^{\mathcal{P}'}_{l'j} = \delta_{l, P_i} A_{ll'} \delta_{l', P'_j} = A_{P_i^{\mathcal{P}}, P'_j^{\mathcal{P}'}} .$$

The inverse matrix of \hat{A} has the property (we use $P^T = P^{-1}$)

$$\hat{A}^{-1} = ((P^{\mathcal{P}})^{-1} A P^{\mathcal{P}'})^{-1} = (P^{\mathcal{P}'})^{-1} A^{-1} P^{\mathcal{P}} \quad (2.66)$$

$$= (P^{\mathcal{P}'})^T A^{-1} P^{\mathcal{P}} \quad (2.67)$$

And consequently,

$$\det(\hat{A}^{-1}) = \det(P^{\mathcal{P}}) \det(P^{\mathcal{P}'}) \det(A^{-1}) . \quad (2.68)$$

2.7.5 Schur complement

We consider the 2×2 block matrix

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

and eliminate the off-diagonal blocks as follows

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ F & \mathbb{1} \end{pmatrix} = \begin{pmatrix} A_{11} + A_{22}F & A_{12} \\ A_{21} + A_{22}F & A_{22} \end{pmatrix}$$

With

$$F = -A_{22}^{-1}A_{21} ,$$

we obtain

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ F & \mathbb{1} \end{pmatrix} = \begin{pmatrix} \tilde{A}_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix}$$

$$\tilde{A}_{11} = A_{11} - A_{12}A_{22}^{-1}A_{21} .$$

Next step:

$$\begin{pmatrix} \mathbb{1} & G \\ 0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} \tilde{A}_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix} = \begin{pmatrix} \tilde{A}_{11} & A_{12} + GA_{22} \\ 0 & A_{22} \end{pmatrix}$$

We use

$$G = -A_{12}A_{22}^{-1}$$

to eliminate the upper right off-diagonal block. Hence

$$\begin{pmatrix} \mathbb{1} & G \\ 0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ F & \mathbb{1} \end{pmatrix} = \begin{pmatrix} \tilde{A}_{11} & 0 \\ 0 & A_{22} \end{pmatrix}$$

Or alternatively

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} \mathbb{1} & -G \\ 0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} \tilde{A}_{11} & 0 \\ 0 & A_{22} \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ -F & \mathbb{1} \end{pmatrix}$$

The determinant is therefore

$$\det(A) = \det(\tilde{A}_{11}) \cdot \det(A_{22}) .$$

and the inverse magtrix

$$A^{-1} = \begin{pmatrix} \mathbb{1} & 0 \\ F & \mathbb{1} \end{pmatrix} \begin{pmatrix} \tilde{A}_{11}^{-1} & 0 \\ 0 & A_{22}^{-1} \end{pmatrix} \begin{pmatrix} \mathbb{1} & G \\ 0 & \mathbb{1} \end{pmatrix}$$

With the 11-block

$$(A^{-1})_{11} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & (A_{22})^{-1} \end{pmatrix} \begin{pmatrix} (\tilde{A}_{11})^{-1} & 0 \\ 0 & (A_{22})^{-1} \end{pmatrix} \begin{pmatrix} \mathbb{1} \\ 0 \end{pmatrix} = (\tilde{A}_{11})^{-1}$$

From which we obtain the relation

$$\begin{aligned} \det (\tilde{A}_{11}^{-1}) &= \det (\tilde{A}_{11})^{-1} = \det \left((A^{-1})_{11} \right) \\ \det (\tilde{A}_{11}) &= \det \left((A^{-1})_{11} \right)^{-1} \end{aligned}$$

and in turn

$$\det (A) = \det \left((A^{-1})_{11} \right)^{-1} \cdot \det (A_{22}) \quad (2.69)$$

$$\frac{\det (A_{22})}{\det (A)} = \det \left((A^{-1})_{11} \right). \quad (2.70)$$

Chapter 3

Real Gases, see additional topics
in the book of Schwabl

Chapter 4

Renormalization Group

4.1 Introduction

We discuss the basic ideas of the renormalization group (RNG) approach in terms of the 1d Ising model

$$H = -J \sum_{i=1}^N s_i s_{i+1} + h' \sum_i s_i , \quad (4.1)$$

as every step can be performed analytically. We assume $N = 2^L$, which allows us to thin out every other spin repeatedly. In addition we assume periodic boundary conditions (pbc), i.e. $s_{N+1} = s_1$. For the partition function we need

$$\tilde{H} := -\beta H := K \sum_i s_i s_{i+1} + h \sum_i s_i + NC , \quad (4.2)$$

where we have added a constant energy NC , as it will become relevant in the renormalization scheme. The pdf for a spin configuration $\{s\}$ then reads

$$\rho_N = \prod_{i=1}^N e^{K s_i s_{i+1} + \frac{h}{2}(s_i + s_{i+1}) + C} \quad (4.3)$$

For later use, we have written the B-field term slightly differently. Next we want to determine the reduced density matrix for the even sites only, which is obtained by the trace over the spins on the odd sites

$$\rho_{\text{even}} = \left(\prod_i^{\text{odd}} \sum_{s_i=\pm 1} \sum_{s_{i+1}=\pm 1} \right) \rho_N \quad (4.4)$$

$$= \left(\prod_i^{\text{even}} e^{h s_i} e^{2C} \right) \left(\prod_i^{\text{odd}} \sum_{s_i=\pm 1} \right) e^{K(s_{i-1} s_i + s_i s_{i+1}) + h s_i} . \quad (4.5)$$

This marginal pdf is required, if we want to calculate the spin-spin correlation for spins on even sites only. In particular, it allows to compute the spin-spin correlation

$$\langle s_{2i} s_{2(i+1)} \rangle . \quad (4.6)$$

If we repeat the marginalization once more, we obtain a marginal pdf that allows to compute

$$\langle s_{4i} s_{4(i+1)} \rangle . \quad (4.7)$$

Hence, the repeated marginalization of half of the sites allows to determine how spin spin-correlations behave on different length scales. Now we want to really compute equation (4.4) [\[previous page\]](#) .

$$\rho_{\text{even}} = \left(\prod_i^{\text{even}} e^{hs_i} e^{2C} \right) \left(\prod_i^{\text{odd}} \sum_{s_i=\pm 1} e^{s_i (K(s_{i-1}+s_{i+1})+h)} \right) \quad (4.8)$$

$$= \left(\prod_i^{\text{even}} e^{hs_i} e^{2C} \right) \left(\prod_i^{\text{odd}} 2 \cosh (K(s_{i-1} + s_{i+1}) + h) \right) \quad (4.9)$$

$$= \prod_i^{\text{even}} e^{hs_i} e^{2C+\ln(2)} \cosh (K(s_i + s_{i+2}) + h) \quad (4.10)$$

$$= \prod_i^{N/2} e^{\frac{h}{2}(s_{2i}+s_{2(i+1)})} e^{2C+\ln(2)} \cosh (K(s_{2i} + s_{2(i+1)}) + h) . \quad (4.11)$$

Next we define $s_i^{(b)} = s_{bi}$ and find in particular for $b = 2$

$$\rho_{\text{even}} = \left(\prod_i^{N/2} e^{\frac{h}{2}(s_i^{(2)}+s_{i+1}^{(2)})} e^{2C+\ln(2)} \cosh (K(s_i^{(2)} + s_{i+1}^{(2)}) + h) \right) . \quad (4.12)$$

Finally, we want to express the marginal density formally identically to equation (4.3)

$$\rho_{\text{even}} := \rho_{N/2} = \prod_{i=1}^{N/2} e^{K' s_i^{(2)} s_{i+1}^{(2)} + \frac{h'}{2}(s_i^{(2)}+s_{i+1}^{(2)})+C'} , \quad (4.13)$$

which is possible, since each factor

$$e^{K' s_i^{(2)} s_{i+1}^{(2)} + \frac{h'}{2}(s_i^{(2)}+s_{i+1}^{(2)})+C'} = e^{\frac{h}{2}(s_i^{(2)}+s_{i+1}^{(2)})+2C+\ln(2)} \cosh (K(s_i^{(2)} + s_{i+1}^{(2)}) + h)$$

only depends on $s_i^{(2)} + s_{i+1}^{(2)}$, and $s_i^{(2)} s_{i+1}^{(2)}$, for which 3 different values are possible each, which defines the 3 parameters K', h', C' . The corresponding conditions are

$$s_i^{(2)} = s_{i+1}^{(2)} = 1 : \quad e^{K'+h'+C'} = e^{h+2C+\ln(2)} \cosh(h+2K) \quad (4.14a)$$

$$s_i^{(2)} = s_{i+1}^{(2)} = -1 : \quad e^{K'-h'+C'} = e^{-h+2C+\ln(2)} \cosh(h-2K) \quad (4.14b)$$

$$s_i^{(2)} = -s_{i+1}^{(2)} : \quad e^{-K'+C'} = e^{2C+\ln(2)} \cosh(h) \quad (4.14c)$$

From equation (4.14c) we obtain

$$e^{C'} = e^{K'+2C+\ln(2)} \cosh(h) \quad (4.15)$$

Insertion in the first two equations yields

$$e^{2K'+h'} \cosh(h) = e^h \cosh(h+2K) \quad (4.16a)$$

$$e^{2K'-h'} \cosh(h) = e^{-h} \cosh(h-2K) . \quad (4.16b)$$

Multiplication of these equations yields

$$e^{4K'} = \frac{\cosh(h+2K) \cosh(h-2K)}{\cosh^2(h)} , \quad (4.17)$$

and division of these equations yields

$$e^{2h'} = e^{2h} \frac{\cosh(h+2K)}{\cosh(h-2K)} . \quad (4.18)$$

equation (4.15) can be written as

$$e^{4C'} = e^{4K'} e^{8C+4\ln(2)} \cosh^4(h) \quad (4.19)$$

Along with equation (4.17) this yields

$$e^{4C'} = \cosh(h+2K) \cosh(h-2K) e^{8C+4\ln(2)} \cosh^2(h) \quad (4.20)$$

The equations 4.17, 4.18, and 4.20 uniquely define the values of h', K', C' , which we now denote as $h^{(2)}, K^{(2)}, C^{(2)}$. The key finding is that the reduced density matrix is formally identical to the original one with modified parameters and due to the translational invariance it is actually the same for the even and odd sites. Therefore we denote it simply by $\rho^{(2)}$. Now we can repeat this procedure and obtain $\rho^{(3)}$, which is the reduced density if only every fourth site is retained. The corresponding parameters are $h^{(3)}, K^{(3)}, C^{(3)}$ and they are related to the parameters $h^{(2)}, K^{(2)}, C^{(2)}$ of the previous iteration

via equation (4.17) , equation (4.18) , and equation (4.20) . In general we obtain the iteration scheme

$$e^{4K^{(n+1)}} = \frac{\cosh(h^{(n)} + 2K^{(n)}) \cosh(h^{(n)} - 2K^{(n)})}{\cosh^2(h^{(n)})} \quad (4.21a)$$

$$e^{2h^{(n+1)}} = e^{2h^{(n)}} \frac{\cosh(h^{(n)} + 2K^{(n)})}{\cosh(h^{(n)} - 2K^{(n)})} \quad (4.21b)$$

$$e^{4C^{(n+1)}} = \cosh(h^{(n)} + 2K^{(n)}) \cosh(h^{(n)} - 2K^{(n)}) e^{8C^{(n)} + 4\ln(2)} \cosh^2(h^{(n)}) . \quad (4.21c)$$

The iteration starts with $K^{(1)} = K, h^{(1)} = h$, and $C^{(1)} = C$. For a first discussion, we consider the case $h = 0$, i.e. no external magnetic field. Then the first iteration yields for h

$$e^{2h^{(2)}} = \frac{\cosh(2K^{(1)})}{\cosh(2K^{(1)})} = 1 , \quad (4.22a)$$

i.e. $h^{(2)} = 0$. Hence, $h^{(n)} = 0$ for all iteration steps. For the parameter K we then obtain the recursion relation

$$e^{4K^{(n+1)}} = \cosh^2(2K^{(n)}) = \frac{1}{4} \left(e^{2K^{(n)}} + e^{-2K^{(n)}} \right)^2 \quad (4.23)$$

$$e^{-4K^{(n+1)}} = \frac{4}{(e^{2K^{(n)}} + e^{-2K^{(n)}})^2} = \frac{4e^{-4K^{(n)}}}{(1 + e^{-4K^{(n)}})^2} \quad (4.24)$$

We introduce the definition $x^{(n)} = e^{-4K^{(n)}}$ for which we obtain

$$x^{(n+1)} = f(x^{(n)})$$

$$f(x) := \frac{4x}{(1+x)^2}$$

The figure illustrates that if we start the recursion with any value $0 < x^{(1)} \leq 1$, i.e. $0 \leq K < \infty$, which corresponds to the parameter of the original physical system, the iteration ends at the fixed point $x^{(\infty)} = 1$. This means that the physical feature (e.g. spin-spin correlation) for very long distances is equivalent to the that of an Ising model with $x = 1$, which corresponds to $K = 0$. This fixed point is called *high temperature fixed point*, as $x = 1$, or rather $K = 0$ is also obtained for $T \rightarrow \infty$ ($\beta \rightarrow 0$). The 1d Ising model considered at very long length scales looks like an infinite temperature or non-interacting solution, which means it is disordered (no long range order). This fixed point is stable or attractive.

The other fixed point $x^* = 0$ is the non-trivial *critical fixed point*. It corresponds to $K = \infty$, i.e. $T = 0$. Here it is the trivial case, without thermal

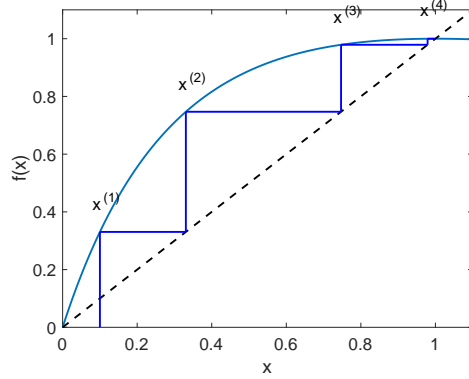


Figure 4.1: **Recursion relation for x in the 1d Ising model. Starting with an arbitrary $x^{(1)} \in (0, 1]$ the fixed point is $x^{(\infty)} = 1$. Only for $x^{(1)} = 0$ the other fixed point $x^{(\infty)} = 0$ is relevant.**

fluctuations, there is long range order, since there are no quantum fluctuations, in contrast to the case of the spin-1/2 Heisenberg model.

Next we study the energy parameter C for the case $h = 0$. Then we have

$$C^{(n+1)} = 2C^{(n)} + \frac{1}{2} \ln \left(\cosh(2K^{(n)}) \right) + \ln(2) . \quad (4.25)$$

As the recursion for $K^{(n)}$ was independent of that for $C^{(n)}$, we can insert the previous result for $K^{(n)}$. Hence for $n \rightarrow \infty$ (very long length scale), we have $K^{(n)} \rightarrow 0$ and we find

$$\begin{aligned} e^{4C^{(n+1)}} &= e^{4(2C^{(n)} + \ln(2))} \\ C^{(n+1)} &= 2C^{(n)} + \ln(2) . \end{aligned}$$

The factor 2 is obvious due to the decimation of the number of spins by the factor 2. The recursion relation for the case $h = 0$ in equation (4.23) [\[previous page\]](#) can also be written as

$$K^{(n+1)} = g(K^n) \quad (4.26)$$

$$g(K) = \left(\frac{1}{2} \ln \left(\cosh(2K) \right) \right) , \quad (4.27)$$

which for large $K^{(n)}$ becomes

$$\begin{aligned} K^{(n+1)} &= \frac{1}{2} \ln \left(\frac{e^{2K^{(n)}} (1 + e^{-4K^{(n)}})}{2} \right) \\ &= K^{(n)} - \frac{\ln(2)}{2} + \ln \left(1 + e^{-4K^{(n)}} \right) . \end{aligned}$$

Hence we have for large $K^{(n)}$

$$K^{(n+1)} \approx K^{(n)} - \frac{\ln(2)}{2} . \quad (4.28)$$

The renormalization group approach can also be used to study how the correlation length depends on β or rather K . If there is no long range order, the correlation length decreases exponentially as

$$\langle s_0 s_m \rangle \sim e^{m/\xi(K)} .$$

The correlation length will depend on $\beta J = K$. In each renormalization step, the unit cell increases by a factor of 2. In the original system we have

$$\langle s_0 s_{2m} \rangle_{K^{(0)}} \sim e^{(2m)/\xi(K^{(0)})} .$$

The same correlation function is equal to that of the renormalized system as follows

$$\langle s_0 s_{2m} \rangle_{K^{(0)}} = \langle s_0^{(2)} s_m^{(2)} \rangle_{K^{(1)}} \sim e^{m/\xi(K^{(1)})} .$$

Comparing the exponentials yields

$$\begin{aligned} \frac{2}{\xi(K^{(0)})} &= \frac{1}{\xi(K^{(1)})} \\ \xi(K^{(1)}) &= \xi(g(K^{(0)})) = \frac{\xi(K^{(0)})}{2} . \end{aligned}$$

Repeating the renormalization m times we obtain the relation

$$\xi(K^{(0)}) = 2^m \xi(g^{(m)}(K^{(0)})) . \quad (4.29)$$

The left hand site is the quantity we are interested in for low temperature or rather $K \gg 1$. In this case, according to equation (4.28) , after m RNG steps we have

$$g^{(m)} K^{(0)} \approx K^{(0)} - \frac{m-1}{2} \ln(2) .$$

If we choose m sufficiently large, eventually, we will reach $K^{(m^*)} = g^{(m^*)} K^{(0)} \sim O(1)$. The required number of steps is

$$m^* \approx \frac{2K^{(0)}}{\ln(2)} .$$

Along with equation (4.29) we obtain

$$\xi(K) = 2^{m^*} \underbrace{\xi(g^{(m^*)}(K))}_{=O(1)} .$$

Now $g(K = O(1))$ is some unimportant constant C and we finally have

$$\xi(K) \sim 2^{m^*} = 2^{\frac{2K}{\ln(2)}} = e^{\ln(2^{\frac{2K}{\ln(2)}})} = e^{2K} .$$

$$\xi(K) \sim e^{2K} . \quad (4.30)$$

So the bottom line is that the correlation length increases exponentially with decreasing temperature in becomes infinite at $T = 0$.

Finally we compute the free energy for $h = 0$. We start out from the partition function for the original system

$$\begin{aligned} Z_N(K, C) &= \text{tr} e^{-\beta H} = \text{tr} e^{K \sum_{\langle ij \rangle} S_i S_j + NC} \\ &= e^{NC} \sum_{\{S_i\}} \prod_{i=0}^{even\ N/2-1} \left\{ \sum_{S_{2i+1}} e^{K S_{2i+1} (S_{2i} + S_{2i+2})} \right\} \\ &= e^{NC} \sum_{\{S_i\}} \prod_{i=0}^{even\ N/2-} \{ 2 \cosh(K(S_{2i} + S_{2i+2})) \} \\ &= Z_{N/2}(K', C') \end{aligned}$$

with K' given in equation (4.26) [p. 93] and C' given in equation (4.25) [p. 93]

$$K^{(1)} = \frac{1}{2} \ln \left(\cosh(2K^{(0)}) \right) \quad (4.31)$$

$$C' = 2C + K^{(1)} + \ln(2) . \quad (4.32)$$

Next we express the partition function slightly different, by pulling C in front

$$Z_N(K, C) = e^{NC} Z_N^{(0)}(K) = e^{\frac{N}{2} C'} Z_{N/2}^{(0)}(K') . \quad (4.33)$$

and taking the logarithm per lattice site (apart from $k_B T$ the free energy per lattice site)

$$\begin{aligned} f(K^{(0)}, C^{(0)}) &= \frac{\ln(Z_N(K^{(0)}, C^{(0)}))}{N} = C^{(0)} + \underbrace{\frac{\ln(Z_N^{(0)}(K^{(0)}))}{N}}_{:=\tilde{f}(K^{(0)})} \\ f(K^{(0)}, C^{(0)}) &= C^{(0)} + \tilde{f}(K^{(0)}) . \end{aligned} \quad (4.34)$$

On the other hand, based on equation (4.33) we obtain

$$\begin{aligned}
 f(K^{(0)}, C^{(0)}) &= \frac{1}{N} \left(\frac{N}{2} C' + \ln(Z_{N/2}^{(0)}(K^{(1)})) \right) \\
 &= \frac{1}{2} C' + \frac{\ln(Z_{N/2}^{(0)}(K^{(1)}))}{N} \\
 &= \frac{1}{2} C' + \frac{1}{2} \frac{\ln(Z_{N/2}^{(0)}(K^{(1)}))}{N/2} \\
 f(K^{(0)}, C^{(0)}) &= \frac{1}{2} \left(C' + \tilde{f}(K^{(1)}) \right)
 \end{aligned}$$

Comparison with equation (4.34) [\[previous page\]](#) yields

$$\tilde{f}(K^{(0)}) = \frac{1}{2} \left(C^{(1)} - 2C^{(0)} + \tilde{f}(K^{(1)}) \right)$$

Inserting equation (4.31) [\[previous page\]](#) finally yields

$$\tilde{f}(K^{(0)}) = \frac{1}{2} \left(K^{(1)} + \ln(2) + \tilde{f}(K^{(1)}) \right) \quad (4.35)$$

A second iteration yields obviously

$$\tilde{f}(K^{(1)}) = \frac{1}{2} \left(K^{(2)} + \ln(2) + \tilde{f}(K^{(2)}) \right) .$$

Inserting in equation (4.35) yields

$$\begin{aligned}
 \tilde{f}(K^{(0)}) &= \frac{1}{2} \left(K^{(1)} + \ln(2) + \frac{1}{2} \left[K^{(2)} + \ln(2) + \tilde{f}(K^{(2)}) \right] \right) \\
 &= \frac{K^{(1)} + \ln(2)}{2^1} + \frac{K^{(2)} + \ln(2)}{2^2} + \frac{\tilde{f}(K^{(2)})}{2^2} .
 \end{aligned}$$

Clearly, this leads after m iterations to

$$\begin{aligned}
 f(K, C) &= \sum_{\nu=1}^m \frac{\ln(2)}{2^\nu} + \sum_{\nu=1}^m \frac{K^{(\nu)}}{2^\nu} + \frac{\tilde{f}(K^{(m)})}{2^m} \\
 &= \ln(2) + \sum_{\nu=1}^m \frac{K^{(\nu)}}{2^\nu} + \frac{\tilde{f}(K^{(m)})}{2^m}
 \end{aligned}$$

We have seen, that $K^{(n)} \rightarrow 0$ for $n \rightarrow \infty$. The partition function for $K \rightarrow 0$ can be obtained analytically as

$$Z_N(K \rightarrow 0) = 2^N ,$$

hence

$$\tilde{f}(K \rightarrow 0) = \frac{\ln(Z_N(K \rightarrow 0))}{N} = \ln(2)$$

So, if we performed an infinite number of renormalization steps, then

$$\begin{aligned} \tilde{f}(K^{(0)}) &= \ln(2) + \sum_{\nu=1}^{\infty} \frac{K^{(\nu)}}{2^{\nu}} + \underbrace{\lim_{L \rightarrow \infty} \frac{\ln(2)}{2^L}}_{=0} \\ &= \ln(2) + \sum_{\nu=1}^{\infty} \frac{K^{(\nu)}}{2^{\nu}} . \end{aligned}$$

We have seen before that the exact result is given by

$$\begin{aligned} Z_N &= d_1^N \\ \tilde{f}(K) &= \ln(d_1) \\ d_1 &= 2 \cosh(K^0) , \end{aligned}$$

Hence, since $C^{(0)} = 0$

$$f(K^{(0)}, C^{(0)}) = \tilde{f}(K^{(0)}) = \ln(2) + \ln(\cosh(K^{(0)})) .$$

Numerical comparison shows the both results agree, i.e.

$$\sum_{\nu=1}^{\infty} \frac{K^{(\nu)}}{2^{\nu}} = \ln(\cosh(K^{(0)}))$$

with

$$K^{(n)} = \frac{1}{2} \ln \left(\cosh(2K^{(n-1)}) \right) .$$

In the 1D case, no approximations were necessary for the RNG procedure.

4.1.1 2D Ising

$$Z_0 := \sum_{S_0} e^{a+hS_0+KS_0\mathcal{S}} = e^a \cdot 2 \cosh(K\mathcal{S} + h) , \quad (4.36)$$

with the abbreviation $\mathcal{S} = S_1 + S_{12} + S_3 + S_4$. The most general exponential form for this expression, since $S_i^2 = 1$, is given by

$$\exp \left(a' + h'\mathcal{S} + K' \sum_{ij} S_i S_j + b \sum_{ijk} S_i S_j S_k + c S_1 S_2 S_3 S_4 \right)$$

In the primed sums no indices are allowed to occur twice and all the indices shall be ordered, e.g. $S_i < S_j < S_k$. We have used the symmetry that equation (4.36) is invariant against interchange of any two indices $i \leftrightarrow j$. The term with 3 spins can equivalently be written as

$$\sum_{ij}^{\prime} S_i S_j = \mathcal{S} \sum_i S_i$$

So we have the constraint

$$a + \ln \left(2 \cosh [K\mathcal{S} + h] \right) = a' + h' \sum_i S_i + K' \sum_{ij}^{\prime} S_i S_j + (b\mathcal{S} + c) S_1 S_2 S_3 S_4 \quad (4.37)$$

Now we consider the possible spin configurations. We begin with $++++$ which yields the condition

$$\begin{aligned} 1) \quad (++++): \quad & a + \ln \left(2 \cosh [4K + h] \right) = a' + 4h' + 6K' + (4b + c) \cdot 1 \\ 2) \quad (++++): \quad & a + \ln \left(2 \cosh [2K + h] \right) = a' + 2h' + 0K' + (2b + c) \cdot (-1) \\ 3) \quad (++++): \quad & a + \ln \left(2 \cosh [0K + h] \right) = a' + 0h' - 2K' + (0b + c) \cdot 1 \end{aligned}$$

Since the geometric position of the spins does not enter in equation (4.37)

2) and 3) are the same if we permute the position of the signs.

The remaining spin configurations are obtained by the transformation $S_i \rightarrow -S_i$, which changes the sign in the terms with an odd number of spins. I.e. 3) is invariant, and for the other two we obtain

$$\begin{aligned} 1') \quad (----): \quad & a + \ln \left(2 \cosh [-4K + h] \right) = a' - 4h' + 6K' + (-4b + c) \cdot 1 \\ 2') \quad (----): \quad & a + \ln \left(2 \cosh [-2K + h] \right) = a' - 2h' + 0K' + (-2b + c) \cdot (-1) \end{aligned}$$

We simplify these equations a bit

$$\begin{aligned}
1) \quad (+ + + +) : \quad & \ln \left(2 \cosh [4K + h] \right) = \Delta a + 4h' + 6K' + 4b + c \\
1') \quad (- - - -) : \quad & \ln \left(2 \cosh [-4K + h] \right) = \Delta a - 4h' + 6K' - 4b + c \\
2) \quad (+ + + -) : \quad & \ln \left(2 \cosh [2K + h] \right) = \Delta a + 2h' - 2b - c \\
2') \quad (- - - +) : \quad & \ln \left(2 \cosh [-2K + h] \right) = \Delta a - 2h' + 2b - c \\
3) \quad (+ + - -) : \quad & \ln \left(2 \cosh [h] \right) = \Delta a - 2K' + c,
\end{aligned}$$

with $\Delta a = a' - a$. We combine the lhs into a column vector \mathbf{d} and likewise for the sought-for parameters $\mathbf{p} = (\Delta a, h', K', b, c)$, resulting in the set of linear equations

$$M\mathbf{p} = \mathbf{d}$$

$$M = \begin{pmatrix} 1 & 4 & 6 & 4 & 1 \\ 1 & -4 & 6 & -4 & 1 \\ 1 & 2 & 0 & -2 & -1 \\ 1 & -2 & 0 & 2 & -1 \\ 1 & 0 & -2 & 0 & 1 \end{pmatrix}$$

If we add or subtract equation 1 and 1' and likewise for 2 and 2', we obtain

$$\begin{aligned}
a) : \quad & \ln \left(4 \cosh [4K + h] \cosh [4K - h] \right) = 2 \left(\Delta a + 6K' + c \right) \\
a') : \quad & \ln \left(\cosh [4K + h] / \cosh [4K - h] \right) = 8(h' + b) \\
b) : \quad & 2 \ln \left(4 \cosh [2K + h] \cosh [2K - h] \right) = 4 \left(\Delta a - c \right) \\
b') : \quad & 2 \ln \left(\cosh [2K + h] / \cosh [2K - h] \right) = 8(h' - b).
\end{aligned}$$

and equation 3) yields

$$c) : \quad \Delta a + c = \ln \left(2 \cosh [h] \right) + 2K',$$

Inserting c) into a) yields

$$\begin{aligned}\tilde{a}) : \quad \ln \left(4 \cosh [4K + h] \cosh [4K - h] \right) &= 2 \ln \left(2 \cosh [h] \right) + 16K' \\ 16K' &= \ln \left(\frac{\cosh [4K + h] \cosh [4K - h]}{\cosh^2([h])} \right)\end{aligned}$$

If we add a') and b') we obtain

$$16h' = \ln \left(\frac{\cosh [4K + h] \cosh^2 [2K + h]}{\cosh [4K - h] \cosh^2 [2K - h]} \right)$$

$$\begin{aligned}e^{-16K'} &= \frac{\cosh^2(h)}{\cosh [4K + h] \cosh [4K - h]} = \frac{(e^h + e^{-h})^2}{(e^{4K+h} + e^{-4K-h})(e^{4K-h} + e^{-4K+h})} \\ &= \frac{e^{2h}(1 + e^{-2h})^2}{e^{8K}e^{2h}(1 + e^{-8K-2h})(e^{-2h} + e^{-8K})} \\ &= e^{-8K} \frac{(1 + e^{-2h})^2}{(1 + e^{-8K-2h})(e^{-2h} + e^{-8K})} \\ e^{-16h'} &= \frac{\cosh [4K - h] \cosh^2 [2K - h]}{\cosh [4K + h] \cosh^2 [2K + h]} \\ &= \frac{(e^{4K-h} + e^{-4K+h})(e^{2K-h} + e^{-2K+h})^2}{(e^{4K+h} + e^{-4K-h})(e^{2K-h} + e^{-2K+h})^2} \\ &= \frac{e^{8K}(e^{-h} + e^{-8K+h})(e^{-h} + e^{-4K+h})^2}{e^{8K}(e^h + e^{-8K-h})(e^{-h} + e^{-4K+h})^2} \\ &= \frac{e^{3h}(e^{-2h} + e^{-8K})(e^{-2h} + e^{-4K})^2}{e^{3h}(1 + e^{-8K-2h})(e^{-2h} + e^{-4K})^2} \\ &= \frac{(e^{-2h} + e^{-8K})(e^{-2h} + e^{-4K})^2}{(1 + e^{-8K-2h})(e^{-2h} + e^{-4K})^2};\end{aligned}$$

$$\begin{aligned}e^{-16K'} &= e^{-8K} \frac{(1 + e^{-2h})^2}{(1 + e^{-8K-2h})(e^{-2h} + e^{-8K})} \\ e^{-16h'} &= \frac{(e^{-2h} + e^{-8K})(e^{-2h} + e^{-4K})^2}{(1 + e^{-8K-2h})(e^{-2h} + e^{-4K})^2};\end{aligned}$$

Especially for $h = 0$ we have

$$\begin{aligned}e^{-16K'} &= e^{-8K} \frac{4^2}{(1 + e^{-8K})(1 + e^{-8K})} \\ e^{-16h'} &= \frac{(1 + e^{-8K})(1 + e^{-4K})^2}{(1 + e^{-8K})(1 + e^{-4K})^2} = 1.\end{aligned}$$

The second equation shows that $h' = 0$. So the renormalized Hamilton function stays field-free. The condition for K' can be written

$$\begin{aligned} K' &= \frac{1}{16} \ln \left(e^{8K} \frac{(1 + e^{-8K})(1 + e^{-8K})}{4} \right) \\ &= \frac{1}{16} \ln \left(\frac{(e^{4K} + e^{-4K})(e^{4K} + e^{-4K})}{4} \right) \\ &= \frac{1}{8} \ln \left(\cosh(4K) \right). \end{aligned}$$

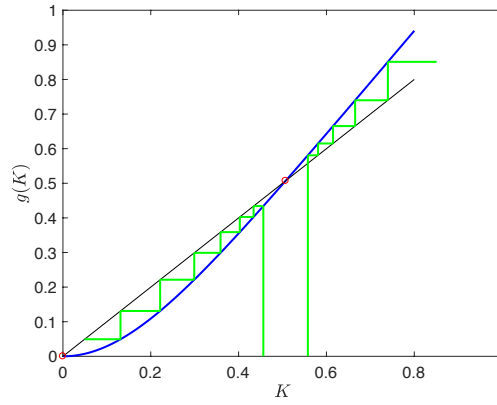


Figure 4.2: **Flux of the renormalization iterations.**

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In figure 4.2 the mapping of the coupling parameter K during the renormalization steps is depicted. We find two fixed points, $K_1^* = 0$ and $K_2^* = 0.507$. The first one is stable, while the second one is unstable. If we start with a physical parameter $K > K_2^*$ the interaction leads to $K = \infty$

We see that the first renormalization step introduces next nearest neighbour interaction as well as interactions involving 4 spins. The later shall be omitted, but we will keep the nnn coupling. So we have to include it. But, as we have seen, starting from $h = 0$ the renormalization steps will not introduce a finite h . So we restrict the discussion to $h = 0$.

Chapter 5

Phase transitions

5.1 Phases

We can generalise the formalism introduced in statistical physics I to incorporate different coexisting phases.

5.1.1 Isolated systems

We begin with isolated systems, where the total volume, total energy, and the partial number per component is conserved. Let's assume that there are N_p coexisting phase, which we enumerate by $(\nu = 1, \dots, N_p)$ and α component, enumerated by $(j = 1, \dots, \alpha)$. The conditions for isolated systems are therefore

$$\sum_{\nu=1}^{N_p} V_\nu = V \quad (5.1a)$$

$$\sum_{\nu=1}^{N_p} U_\nu = U \quad (5.1b)$$

$$\sum_{\nu=1}^{N_p} N_{j\nu} = N_j, \text{ for } j = 1, \dots, \alpha. \quad (5.1c)$$

Here V_ν (U_ν) is the total volume (energy) of the particles in phase ν . N_j is the total number of particles of component j and $N_{j\nu}$ the number of component j that is in phase ν . We also introduce the following vectors

$$\mathbf{N} = (N_{j=1}, N_{j=1}, \dots, N_\alpha)^T \quad (5.2)$$

$$\mathbf{N}_\nu = (N_{j=1,\nu}, N_{j=1,\nu}, \dots, N_{\alpha,\nu})^T. \quad (5.3)$$

The entropy as extensive quantity is

$$S(U, V, \mathbf{N}) = \sum_{\nu=1}^{N_p} S_{\nu}(U_{\nu}, V_{\nu}, \mathbf{N}_{\nu}) \quad (5.4)$$

For an isolated system (micro-canonical ensemble) the entropy represents the thermodynamic potential and in equilibrium it has to be maximal. So we have to maximize the entropy based on the constraints in equation (5.1) [\[previous page\]](#). This is best achieved by Lagrange multipliers, i.e. we define

$$\mathcal{L} = \sum_{\nu} S_{\nu}(U_{\nu}, V_{\nu}, \mathbf{N}_{\nu}) - \lambda^V \sum_{\nu} V_{\nu} - \lambda^U \sum_{\nu} U_{\nu} - \sum_j \lambda_j^N \sum_{\nu} N_{j\nu} \quad (5.5)$$

and form the differential

$$d\mathcal{L} = \sum_{\nu=1}^{N_p} \left[\left. \frac{\partial}{\partial U_{\nu}} S_{\nu}(U_{\nu}, V_{\nu}, \mathbf{N}_{\nu}) \right|_{V_{\nu}, \mathbf{N}_{\nu}} - \lambda^U \right] dU_{\nu} \quad (5.6a)$$

$$+ \sum_{\nu=1}^{N_p} \left[\left. \frac{\partial}{\partial V_{\nu}} S_{\nu}(U_{\nu}, V_{\nu}, \mathbf{N}_{\nu}) \right|_{U_{\nu}, \mathbf{N}_{\nu}} - \lambda^V \right] dV_{\nu} \quad (5.6b)$$

$$+ \sum_{\nu=1}^{N_p} \sum_{j=1}^{\alpha} \left[\left. \frac{\partial}{\partial N_{j\nu}} S_{\nu}(U_{\nu}, V_{\nu}, \mathbf{N}_{\nu}) \right|_{U_{\nu}, V_{\nu}, N_{i\nu}, i \neq j} - \lambda_j^N \right] dN_{j\nu} \stackrel{!}{=} 0. \quad (5.6c)$$

First of all, the variations in volume, energy, and particle number are independent from each other and, therefore, we have the individual conditions

$$\sum_{\nu=1}^{N_p} \left[\left. \frac{\partial}{\partial U_{\nu}} S_{\nu}(U_{\nu}, V_{\nu}, \mathbf{N}_{\nu}) \right|_{U_{\nu}, \mathbf{N}_{\nu}} - \lambda^U \right] dU_{\nu} = 0 \quad (5.7a)$$

$$\sum_{\nu=1}^{N_p} \left[\left. \frac{\partial}{\partial V_{\nu}} S_{\nu}(U_{\nu}, V_{\nu}, \mathbf{N}_{\nu}) \right|_{U_{\nu}, \mathbf{N}_{\nu}} - \lambda^V \right] dV_{\nu} = 0 \quad (5.7b)$$

$$\sum_{\nu=1}^{N_p} \sum_{j=1}^{\alpha} \left[\left. \frac{\partial}{\partial N_{j\nu}} S_{\nu}(U_{\nu}, V_{\nu}, \mathbf{N}_{\nu}) \right|_{U_{\nu}, V_{\nu}, N_{i\nu}, i \neq j} - \lambda_j^N \right] dN_{j\nu} = 0. \quad (5.7c)$$

According to the constraints equation (5.1) [\[previous page\]](#), there is one condition for the variables U_{ν} , i.e. we can choose U_{ν} for $\nu = 1, 2, \dots, N_p - 1$ as we like and U_{N_p} follows from the constraint. Then we can always demand that

$$\lambda^U = \left. \frac{\partial}{\partial U_{N_p}} S_{N_p}(U_{N_p}, V_{N_p}, \mathbf{N}_{N_p}) \right|_{U_{N_p}, \mathbf{N}_{N_p}}, \quad (5.8)$$

as long as we are eventually able to fulfil the constraint equation (5.7a) . Then the remaining constraint reads

$$\sum_{\nu=1}^{N_p-1} \left[\frac{\partial}{\partial U_\nu} S_\nu(U_\nu, V_\nu, \mathbf{N}_\nu) - \lambda^U \right] dU_\nu = 0; .$$

Here all dU_ν are independent and the square brackets have to vanish individually. In total we have

$$\lambda^U = \frac{\partial}{\partial U_\nu} S_\nu(U_\nu, V_\nu, \mathbf{N}_\nu) \Big|_{V_\nu, \mathbf{N}_\nu} = \frac{1}{T_\nu} . \quad (5.9a)$$

Similarly, we obtain from the other constraints

$$\lambda^V = \frac{\partial}{\partial V_\nu} S_\nu(U_\nu, V_\nu, \mathbf{N}_\nu) \Big|_{U_\nu, \mathbf{N}_\nu} = \frac{p_\nu}{T_\nu} . \quad (5.9b)$$

and

$$\frac{\partial}{\partial N_{j\nu}} \lambda_j^V = S_\nu(U_\nu, V_\nu, \mathbf{N}_\nu) \Big|_{U_\nu, V_\nu, N_{i\nu}, i \neq j} = -\frac{\mu_{j\nu}}{T_\nu} , \quad \text{for } j = 1, \dots, \alpha . \quad (5.9c)$$

So we find that in an isolated system in equilibrium all phases have the same temperature T , the same pressure p and the same chemical potential μ_j for component j . But in general, we still have $\mu_j \neq \mu_{j'}$.

5.1.2 Closed system with $p = \text{fixed}$, $T = \text{fixed}$

Another important system is that where pressure and temperature are fixed experimentally. In this case the Free Enthalphy $G(p, T, \mathbf{N})$ is the relevant thermodynamic potential. The equilibrium condition is G has to be minimal, or rather $dG = 0$. Again G is extensive, i.e. additive w.r.t. the phases

$$G = \sum_{\nu=1}^{N_p} G_\nu(T, p, \mathbf{N}_\nu) \quad (5.10)$$

Here, we have already exploited that all phases have the same temperature and pressure, which is given at the outset. So the only d.o.f. that can be varied are the particle numbers, still under the constrain, used before. A similar derivation now yields

$$\lambda_j^N = \frac{\partial}{\partial N_{j\nu}} G_\nu(T, p, \mathbf{N}_\nu) \Big|_{T, p, N_{i\nu}, i \neq j} = \mu_{j,\nu} . \quad (5.11)$$

and we find that in closed system, where T and p is fixed, the chemical potential of component j is the same in all phases.

5.1.3 Number of degrees of freedom

The chemical potentials will depend on T , p , and in principle on the particle numbers

$$\mu_{j\nu} = \mu_{j\nu}(T, p, \{N_{j\nu}\}) \quad (5.12)$$

Now, the chemical potentials are intensive quantities, i.e. scaling the extensive quantities in its argument, by a common factor does not change the chemical potential. Let's consider an intensive function f that shall depend on T , p , and some particle numbers N_l . Scaling the total size by λ results in particle numbers λN_l . As T and p are intensive, we have

$$f(T, p, \{\lambda N_l\}) = f(T, p, \{N_l\}) .$$

This is the case if f only depends on the concentrations $c_j = N_j / \sum_i N_i$, since scaling all N_j by a common factor does not change the concentration. By phase we mean a spatial area within which no abrupt changes of any physical quantity occur, but at the boundary of which such changes can be observed. The system consists of one or more components/ component. Component means the minimum number of independent chemical substances that we need to produce the phase. The state of the system is described by a number of state variables depending on the type of system. By degrees of freedom F we mean the number of state variables that we can vary independently of each other without any of the phases disappearing. First of all, we want to assume that no chemical reactions take place in the system. The state of each phase is clearly defined when we specify T , p , and the mole fraction of component j in phase ν .

$$c_j^{(\nu)} := \frac{N_{j\nu}}{N_\nu} \quad (5.13)$$

i.e. the fraction of particles in phase ν that belong to component j . Then

$$\sum_j c_j^{(\nu)} = 1 , \quad \forall \nu . \quad (5.14)$$

Scaling the total size of the system by a common factor λ , i.e. in particular $N_{j\nu} \rightarrow \lambda N_{j\nu}$, does not change the phases. So along with the intensivity of the chemical potentials, we know by now that the latter depend on the mole fractions and not the absolute particle numbers

$$\mu_{j\nu} = \mu_{j\nu}(T, p, \{c_j^{(\nu)}\}) \quad (5.15)$$

The number of state variables is $Z_\nu = 2 + \alpha N_\nu$, but they are not independent. According to equation (5.11) [\[previous page\]](#) we have the equilibrium

conditions, which include the conditions for the particle numbers in equation (5.1c) [\[p. 102\]](#)

$$\mu_{j\nu}(T, p, \{N_{j\nu}\}) = \mu_{j\nu'}(T, p, \{N_{j\nu}\}) , \forall \nu \neq \nu' \text{ and } \forall j .$$

These are $N_p - 1$ conditions for each component, i.e. in total $\alpha(N_p - 1)$ constraints. In addition we have the N_p normalization constraints in equation (5.14) [\[previous page\]](#) . So the total number of constraints is

$$Z_c = \alpha N_p - \alpha + N_p ,$$

and therefore the number of d.o.f. is the number of state variables minus the number of constraints resulting in

GIBBS' PHASE RULE	
$f = 2 + \alpha - N_p .$	(5.16)

Example: H_2O Phase diagram

For water: $T_{tp} = 273, 16000K(0, 01000C)$, $p_{tp} = 611, 657Pa$. $T_c = 647.096K$, $p_c = 22.064MPa$ and $\rho_c = 356kg/m^3$.

solid-liquid: melting, freezing

liquid-gas: condensation, vaporization

solid-gas: sublimation, deposition

Anomaly of water: increasing reduces the volume and the density increases. By increasing pressure, solid water becomes liquid. Hence, the density of solid water (ice) is smaller than of liquid water. That is the reason why ice floats on water.

What is a one component liquid, i.e. $\alpha = 1$.

Pure phase (solid,liquid,gas), $N_p = 1$

The number of d.o.f. is

$$f = 2 + 1 - 1 = 2 ,$$

which means we can vary T and p independently.

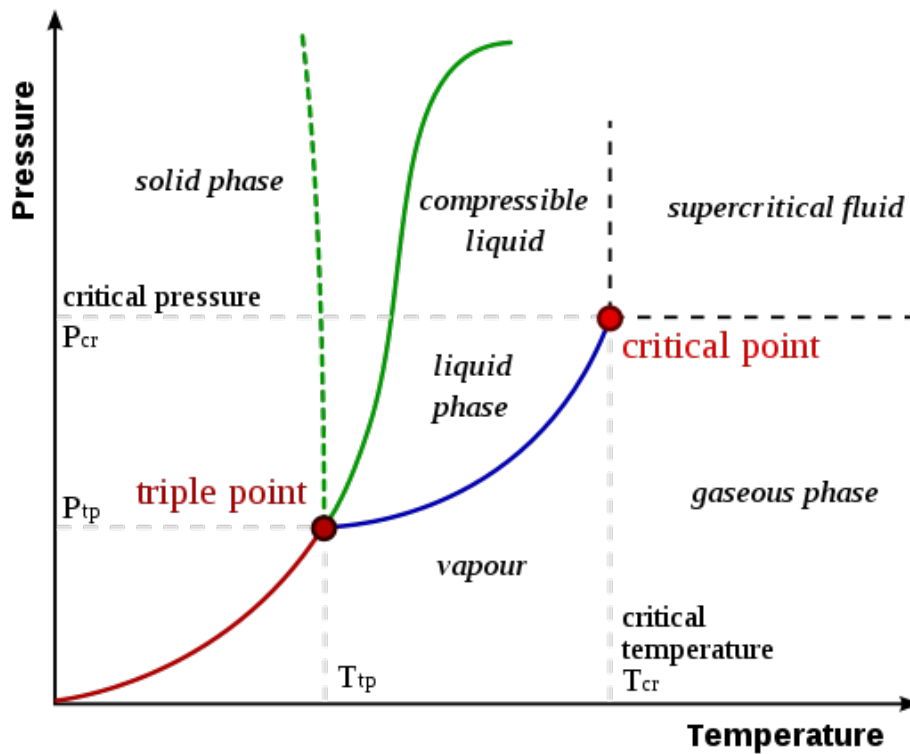


Figure 5.1: Phase diagram of water, taken from 'wikipedia'. The dashed green line is the melting-point line of water (negative slope, anomalous). The solid green line is the melting-point line of most other substances (positive slope, normal).

Two coexisting phases, $N_p = 2$

- boiling curve (liquid to gas)
- condensation curve (liquid to gas)
- melting curve (solid to liquid)
- solidification curve (liquid to solid)
- sublimation curve (solid to gas)
- resublimation curve (gas to solid)

melting-point line (solid to liquid) Condensation curve () Siedekurve (liquid to gas)

sublimation (solid to gas) resublimation (gas to solid)

The number of d.o.f. is

$$f = 2 + 1 - 2 = 1 ,$$

which means, we have to vary T and p on a curve, $p(T)$, e.g. melting-point line.

Three coexisting phases, $N_p = 3$, triple point

Here $f = 0$. There is no degree of freedom.

It also follows, that for a one-component substance there are at most 3 phases, otherwise the number of d.o.f. become negative.

5.1.4 Clausius-Clapeyron

As a further application of the previous discussion, we consider the coexistence line between liquid and gas (Condensation curve) of a one-component system, such as water.

If we choose T and P as the two independent d.o.f. then according to equation (5.11) [p. 104] we have

$$\mu_{fl}(T, p) = \mu_g(T, p) . \quad (5.17)$$

This relation allows to determine the condensation curve $p(T)$ on which the fluid and the gas phase coexist. Away from this curve, only one phase exists, namely the one where the chemical potential is smaller. This is due to the Gibbs-Duhem relation

$$G(T, p, N) = \mu N .$$

In the case of a single phase, the system will minimize the Free Enthalpy. Since N is fixed, the phase with the smaller chemical potential has a smaller Free Enthalpy.

The free Enthalpy is related to the free energy $F(T, V, N)$ via a Legendre transformation, where V is replaced by p . We start out with

$$\left. \frac{\partial}{\partial V} F(T, V, N) \right|_{T, N} = -p$$

This relation can be inverted for given T, N and p we obtain

$$V = V(p, T, N)$$

$$G(T, p, N) = F(T, V(p, T, N), N) + pV . \quad (5.18)$$

Then

$$\begin{aligned} dG &= dF + pdV + Vdp \\ &= -SdT - pdV + \mu dN + pdV + Vdp \\ dG &= -SdT + \mu dN + Vdp . \end{aligned}$$

Furthermore we have seen before

$$dG = \mu dN - SdT + Vdp ,$$

or rather

$$dG - \mu dN = -SdT + Vdp .$$

On the other hand the Gibbs-Duhem relation yields

$$dG = \mu dN + Nd\mu \Rightarrow dG - \mu dN = Nd\mu .$$

Combining the two relation yields

$$-SdT + Vdp = Nd\mu .$$

This is generally valid and it also applies individually to different phases, i.e.

$$\begin{aligned} -S_\nu dT + V_\nu dp &= N_\nu d\mu_\nu \\ -\frac{S_\nu}{N_\nu} dT + \frac{V_\nu}{N_\nu} dp &= d\mu_\nu . \end{aligned}$$

We introduce entropy and volume per particle

$$s_\nu = \frac{S_\nu}{N_\nu} \quad (5.19)$$

$$v_\nu = \frac{V_\nu}{N_\nu} , \quad (5.20)$$

and obtain

$$-s_\nu dT + v_\nu dp = d\mu_\nu . \quad (5.21)$$

Now we consider changes dp, dT along the coexistence line. There we have due to equation (5.17) [\[previous page\]](#)

$$d\mu_{fl}(T, p) = d\mu_g(T, p) .$$

Along with equation (5.21) we obtain

$$\begin{aligned} -s_{fl}dT + v_{fl}dp &= -s_gdT + v_gdp \\ \frac{dp}{dT} &= \frac{s_g - s_{fl}}{v_g - v_{fl}} = \frac{\Delta s}{\Delta v} . \end{aligned}$$

Finally, we define the molar vaporation enthalpy

$$q = T(s_g - s_{fl})$$

and find the

CLASIUS-CLAPEYRON RELATION	
$\frac{dp}{dT} = \frac{q}{T(v_g - v_{fl})} .$	(5.22)

In the derivation of the Clausius-Clapeyron relation we have assumed that $S_g \neq S_{fl}$ and $V_g \neq V_{fl}$, which means, although

$$\mu_g(T, p) = \mu_{fl}(T, p)$$

that

$$\begin{aligned} \left. \frac{\partial \mu_g}{\partial T} \right|_p &\neq \left. \frac{\partial \mu_{fl}}{\partial T} \right|_p \\ \left. \frac{\partial \mu_g}{\partial p} \right|_T &\neq \left. \frac{\partial \mu_{fl}}{\partial p} \right|_T . \end{aligned}$$

Such a phase transition is a first order phase transition.

The Clausius-Clapeyron relation is only valid for first order phase transitions.

5.1.5 Real gases (van der Waals equation)

In an earlier chapter we have discussed the ideal gas and its equation of state

$$pV = Nk_B T .$$

We also introduced finite eigen-volumes of the molecules and obtained

$$p(V - V_0) = Nk_B T .$$

Finally, we also want to include the intermolecular forces. For molecules in the bulk of the material, these forces vanish on average, as they act with equal strength in opposite directions. This is not the case in the surface layer, where the partners outside the surface are missing. This results in an effective force, pulling the molecules in the surface layer into the bulk. I.e. the intermolecular forces act at the surface like an additional pressure (internal pressure). It has the form

$$a \frac{N^2}{V^2}$$

resulting in

VAN DER WAALS EQUATION (<i>extensive form</i>)
$\left(p + a' \frac{N^2}{V^2} \right) \left(V - \overbrace{Nb'}^{V_0} \right) = Nk_B T . \quad (5.23)$

It can also be expressed in term of molar volume v , pressure and temperature, i.e. the intensive form

VAN DER WAALS EQUATION (<i>intensive representation</i>)
$\left(p + \frac{a'}{v^2} \right) (v - b') = k_B T . \quad (5.24)$

Here, b' is the eigen-volume of one molecule.

We multiply equation (5.24) [\[previous page\]](#) by v^2 and find that it becomes a cubic equation in v

$$\begin{aligned} (pv^2 + a')(v - b') - k_B T v^2 &= 0 \\ pv^3 + a'v - b'pv^2 - a'b' - k_B T v^2 &= 0 . \end{aligned}$$

Next we introduce suitable units p_{cr}, v_{cr}, T_{cr} and the corresponding dimensionless quantities π, ν, t via

$$\begin{aligned} p &= \pi p_{cr} \\ v &= \nu v_{cr} \\ T &= t T_{cr} , \end{aligned}$$

resulting in

$$\begin{aligned} \pi \nu^3 + \frac{a' v_{cr}}{p_{cr} v_{cr}^3} \nu - \frac{b' p_{cr} v_{cr}^2}{p_{cr} v_{cr}^3} \pi \nu^2 - \frac{a' b'}{p_{cr} v_{cr}^3} - \frac{k_B T_{cr} v_{cr}^2}{p_{cr} v_{cr}^3} t \nu^2 &= 0 \\ \pi \nu^3 + \underbrace{\left(\frac{a'}{p_{cr} v_{cr}^2} \right)}_{=T_1} \nu - \underbrace{\left(\frac{b'}{v_{cr}} \right)}_{=T_2} \pi \nu^2 - \underbrace{\left(\frac{a' b'}{p_{cr} v_{cr}^3} \right)}_{=T_3} - \underbrace{\left(\frac{k_B T_{cr}}{p_{cr} v_{cr}} \right)}_{=T_4} t \nu^2 &= 0 \\ \pi \nu^3 + T_1 \nu - T_2 \pi \nu^2 - T_3 - \underbrace{\left(\frac{k_B T_{cr}}{p_{cr} v_{cr}} \right)}_{=T_4} t \nu^2 &= 0 . \end{aligned}$$

Now we have the freedom to choose the parameters p_{cr}, v_{cr} , and T_{cr} suitably. We use

$$T_2 = \left(\frac{b'}{v_{cr}} \right) = \frac{1}{3} \tag{5.25}$$

$$T_3 = \left(\frac{a' b'}{p_{cr} v_{cr}^3} \right) = 1 \tag{5.26}$$

$$T_4 = \left(\frac{k_B T_{cr}}{p_{cr} v_{cr}} \right) = \frac{8}{3} \tag{5.27}$$

then

CRITICAL VALUES
(*van der Waals*)

$$v_{cr} = 3b' \quad (5.28)$$

$$\Rightarrow p_{cr} = \frac{a'b'}{v_{cr}^3} = \frac{a'}{27b'^2} \quad (5.29)$$

$$\Rightarrow T_1 = \frac{a'}{p_{cr}v_{cr}^2} = \frac{a'}{\frac{a'}{27b'^2}9b'^2} = 3 \quad (5.30)$$

$$k_B T_{cr} = \frac{8}{3} p_{cr} v_{cr} = \frac{8}{3} \frac{a'}{27b'^2} 3b' = \frac{8a'}{27b'} . \quad (5.31)$$

So we have

$$\pi\nu^3 + 3\nu - \frac{\pi\nu^2}{3} - 1 = \frac{8}{3}t\nu^2 \quad (5.32)$$

$$\left(\pi + \frac{3}{\nu^2}\right)\left(\nu - \frac{1}{3}\right) = \frac{8}{3}t . \quad (5.33)$$

Solving for π yields

$$\pi = \frac{8t}{3\nu - 1} - \frac{3}{\nu^2}$$

The term $(3\nu - 1)$ originated from $V - V_0$, and therefore it is always positive, as the total volume has to be greater than the eigenvolume.

If we plot $\pi(\nu)$ for fixed t (isotherm) then we find different behaviour for $t < 1$, $t = 1$ and $t > 1$.

- For $t < 1$ the curve has a minimum and a maximum in the physical interval $\nu > 1/3$.
- For $t = 1$ minimum and maximum coincide at $\nu = 1$, with $\pi(\nu = 1) = 1$.
- For $t > 1$ the curve is monotonically decreasing in the physical interval.

As we will see soon, if the curve has a maximum and a minimum then there is a phase transition. If it is monotonically decreasing, there is no phase transition. Hence, the parameters p_{cr} , v_{cr} , and T_{cr} represent the critical point.

Inserting the critical values into the equation of state for the ideal gas in form of the following ratio then we obtain

$$Z := \frac{p_{cr} v_{cr}}{k_B T_{cr}} = \frac{\frac{a'}{27b'^2} 3b'}{\frac{8a'}{27b'}} = \frac{3}{8} . \quad (5.34)$$

Experimentally one finds for all real gases am kritischen Punkt $Z < 3/8$, while the ideal gas yields $Z = 1$. In this respect the van der Waals model is clearly better. Alternatively, equation (5.34) can be written with $\rho_c = 1/v_{cr}$ as

$$p_{cr} = \frac{3}{8} k_B T_{cr} \rho_{cr} . \quad (5.35)$$

5.1.6 Maxwell-Construction

We have just seen that the equation of state for the van der Waals model read in dimensionless units i

$$\left(\pi - \frac{3}{\nu^2} \right) \left(\nu - \frac{1}{3} \right) = \frac{8}{3} t .$$

As we have seen, for $t < 1$ there are regions in the $\pi - \nu$ -diagramm where the isotherm compressibility

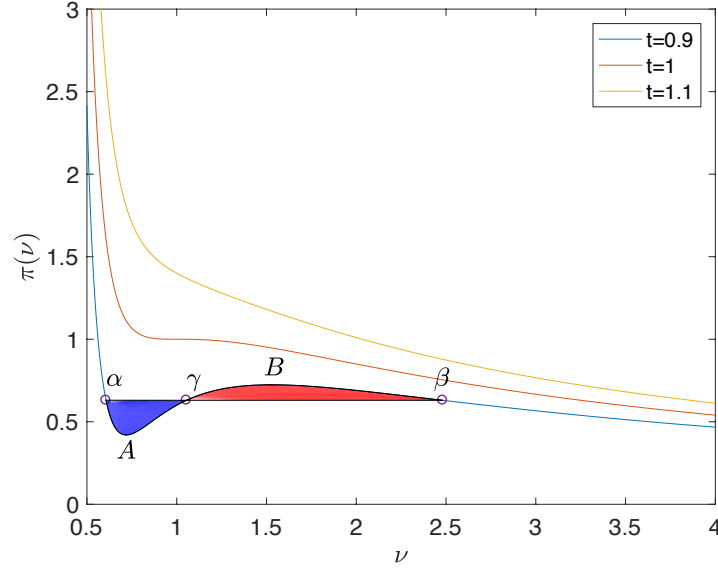
$$\kappa_T = -\frac{1}{V} \left(\frac{\partial V}{\partial p} \Big|_T \right) = -\frac{1}{p_{cr} \nu} \left(\frac{\partial \nu}{\partial \pi} \Big|_T \right) < 0 \quad (5.36)$$

becomes negative. This implies that the system is mechanically unstable, it would shrink by itself. The reason is that the van der Waals model describes a single phase of a one-component system. It is applicable for large volume, in the gas phase, and for small volume, in the liquid phase, but in between there is a phase transition, where 2 phases coexist, which cannot be described by the vdW equation. What happens in reality is the following. We have seen before that generally in the coexistence line between liquid and gas, the number of d.o.f. is merely 1 and it is describe d by $p = p(T)$. On isotherms, T is fixed and hence p is fixed.

In the pV-diagram all isotherms for ($T < T_c$) in the two-phase region are horizontal lines.

We denote the pressure on the coexistence line by $p_{\alpha\beta}$. In the pure phase regions the vdW model is still valid. we have the condition

$$\mu_{fl}(T, p) = \mu_g(T, p) ,$$

Figure 5.2: **Maxwell construction.**

i.e. pressure is a function of temperature alone and independent of the volume. Hence for the isotherm compression, discussed before, the pressure in when reducing the volume in the two-phase region, does not change

In the coexistence region we have

$$\mu_{fl}(T, P_{\alpha\beta}) = \mu_g(T, P_{\alpha\beta})$$

In addition, at the points α and β , we have pure phases and therefore $N_\alpha = N$ and $N_\beta = N$ and consequently

$$\mu_{fl}(T, P_{\alpha\beta})N_\alpha = \mu_g(T, P_{\alpha\beta})N_\beta$$

The Gibbs-Duhem relation then yields

$$\begin{aligned} G_\alpha &= G_\beta \\ F_\alpha + p_\alpha V_\alpha &= F_\beta + p_\beta V_\beta \end{aligned}$$

or rather

$$F_\alpha - F_\beta = -p_{\alpha\beta}(V_\alpha - V_\beta) . \quad (5.37)$$

This is the result, if we assume a coexistence of two phases. Alternatively, if we stick to one phase then the vdW equation determines the pressure curve,

the one given in figure 5.2 with the wavy look. In that case, the differential of the free energy is, since N is fixed and T is fixed (isotherm),

$$dF = SdT - pdV + \mu dN = -pdV ,$$

and the integral yields

$$F_\alpha - F_\beta = \int_\beta^\alpha dF = - \int_{V_\beta}^{V_\alpha} p(T, V', N) dV' .$$

$$F_\alpha - F_\beta = \int_{V_\alpha}^{V_\beta} p(T, V', N) dV' \quad (5.38)$$

By combining equation (5.37) [\[previous page\]](#) and equation (5.38) we find

$$\int_{V_\alpha}^{V_\beta} p(T, V', N) dV' = p_{\alpha\beta} (V_\beta - V_\alpha) \quad (5.39)$$

I.e., the area under the vdW curve $p(t, V, N)$ in the interval (V_α, V_β) has to be same as the area of the $p(V) = p_{\alpha\beta}$ curve in the two-phase region. Consequently, the subareas A and B have to be same.

Finally, we will show that the pure phase is unstable w.r.t. to the mixed phase. To this end we compare two states with the same T and V but different pressures $p_{\alpha\beta}$ the vdW pressure $p(T, V, N)$. Since T and V is fixed, we have to compare the free energies.

In the pure phase compute the free energy for a given V in the interval (V_α, V_β) . To this end we use $dF = -pdV$ and integrate from V_α to V

$$F_{vdW}(V, T) = F_\alpha - \int_{V_\alpha}^V p(V', T) dV' . \quad (5.40)$$

In the two-phase region the free energy is the linear combination of the free energy of the two phases according to their relative size, i.e.

$$F_{mp} = c_{fl} F_{fl} + c_g F_g \quad (5.41)$$

$$= c_{fl} F_\alpha + c_g F_\beta , \quad (5.42)$$

with $c_{fl} = N_{fl}/N$ and $c_g = N_g/N$, hence $c_{fl} + c_g = 1$. Then

$$\begin{aligned} F_{mp} &= F_\alpha + (c_{fl} - 1)F_\alpha + c_g F_\beta \\ &= F_\alpha - c_g F_\alpha + c_g F_\beta \\ F_{mp} &= F_\alpha + c_g (F_\beta - F_\alpha) . \end{aligned} \quad (5.43)$$

Finally, we want to express c_g in terms of volume. The total volume is split accordingly,

$$\begin{aligned} V &= c_{fl}V_{fl} + c_gV_g = (1 - c_g)V_\alpha + c_gV_\beta \\ V - V_\alpha &= c_g(V_\beta - V_\alpha) \end{aligned}$$

and we obtain the relative portions of the phases

$$c_g = \frac{V - V_\alpha}{V_\beta - V_\alpha} \quad (5.44a)$$

$$c_{fl} = \frac{V_\beta - V}{V_\beta - V_\alpha} . \quad (5.44b)$$

We then have

$$F_{mp} = F_\alpha + \frac{V - V_\alpha}{V_\beta - V_\alpha}(F_\beta - F_\alpha) . \quad (5.45)$$

Here we can also use equation (5.37) [\[p. 115\]](#) resulting in

$$F_{mp} = F_\alpha - p_{\alpha\beta} \frac{V - V_\alpha}{V_\beta - V_\alpha}(V_\beta - V_\alpha) = F_\alpha + p_{\alpha\beta}(V - V_\alpha) \quad (5.46)$$

The difference of the free energies is according to equation (5.40) [\[previous page\]](#) and equation (5.46)

$$F_{vdW}(V, T) - F_{mp}(V, T) = p_{\alpha\beta}(V - V_\alpha) - \int_{V_\alpha}^V p(V', T) dV' \geq 0$$

The reason can be seen in figure 5.2. As long as $V \in (V_\alpha, V_\gamma)$ it is obvious that the integral over $p(V', T)$ is smaller than the area of the rectangle formed obtained if p is replaced by $p_{\alpha\beta}$. For $V > V_\gamma$ we can modify the equation as follows

$$\begin{aligned} F_{vdW}(V, T) - F_{mp}(V, T) &= p_{\alpha\beta}(V_\gamma - V_\alpha) + p_{\alpha\beta}(V - V_\gamma) - \left(\int_{V_\alpha}^{V_\gamma} p(V', T) dV' + \int_{V_\gamma}^V p(V', T) dV' \right) \\ &= p_{\alpha\beta}(V_\gamma - V_\alpha) - \underbrace{\int_{V_\alpha}^{V_\gamma} p(V', T) dV'}_{=A} - \int_{V_\gamma}^V (p(V', T) - p_{\alpha\beta}) dV' \end{aligned}$$

For $V \in (V_\gamma, V_\beta)$ the integrand is positive and

$$\int_{V_\gamma}^V (p(V', T) - p_{\alpha\beta}) dV' \leq B$$

since B is the value of the integral over the entire interval (V_γ, V_β) . According to the Maxwell construction $B = A$, hence the integral is less than A so in total we find

$$F_{vdW}(V, T) - F_{mp}(V, T) \geq 0 ,$$

as we have claimed before.

5.2 Phasetransitions

In case of the liquid-gas mixture we have seen that the transition occurs at fixed T and fixed p , the latter is

$$p_{\alpha,\beta}(T) : \quad \text{vapor pressure}$$

In the transition region we have a mixture of the liquid and the gas state. The percentage portion is given by equation (5.44) [\[previous page\]](#).

The supplied heat leads to transformation of a fraction of the fluid into gas. This process is isotherm, since heat is only used to overcome the binding energy present in the fluid. Only if the entire fluid is vaporized, further heat transfer results in a temperature rise. Heat transfer that occurs at a constant system temperature but changes the state variable is called latent heat with respect to the variable.

Such phase transitions, that involve *latent heat* are *first order phase transitions*. *Latent heat* in contrast to *sensible heat* does not lead to a change in temperature.

Only for first order phase transitions, the Clausius-Clapeyron equation is applicable, as it requires that entropy and volume per particle are different in the two phases.

We recall that

$$S = - \left. \frac{\partial G}{\partial T} \right|_p \quad (5.47)$$

$$V = - \left. \frac{\partial G}{\partial p} \right|_T . \quad (5.48)$$

A characteristic feature of first order phase transition is discontinuity of the **first** derivative of the thermodynamic potential when crossing the coexistence line in the phase diagram. Along the line it is continuous.

Next we exploit in addition the following relations

$$S = -\left.\frac{\partial F}{\partial T}\right|_V, \quad (5.49)$$

$$p = -\left.\frac{\partial F}{\partial V}\right|_T. \quad (5.50)$$

which allow to compute specific heat and compressibility in term of the free enthalpy or free energy

$$0 \leq C_p = T \left.\frac{\partial S}{\partial T}\right|_p = -T \left.\frac{\partial^2 G}{\partial T^2}\right|_p \Rightarrow \left.\frac{\partial^2 G}{\partial T^2}\right|_p \leq 0 \quad (5.51)$$

$$0 \leq \kappa_T = -\frac{1}{V} \left.\frac{\partial V}{\partial p}\right|_T = -\frac{1}{V} \left.\frac{\partial^2 G}{\partial p^2}\right|_T \Rightarrow \left.\frac{\partial^2 G}{\partial p^2}\right|_T \leq 0 \quad (5.52)$$

$$0 \leq C_V = T \left.\frac{\partial S}{\partial T}\right|_V = -T \left.\frac{\partial^2 F}{\partial T^2}\right|_V \Rightarrow \left.\frac{\partial^2 F}{\partial T^2}\right|_V \leq 0 \quad (5.53)$$

$$0 \leq \frac{1}{\kappa_T} = -V \left.\frac{\partial p}{\partial V}\right|_T = V \left.\frac{\partial^2 F}{\partial V^2}\right|_T \Rightarrow \left.\frac{\partial^2 F}{\partial V^2}\right|_T \geq 0. \quad (5.54)$$

Hence we have

$$\left.\frac{\partial^2 G}{\partial T^2}\right|_p \leq 0 \quad \left.\frac{\partial^2 G}{\partial p^2}\right|_T \leq 0 \quad (5.55)$$

$$\left.\frac{\partial^2 F}{\partial T^2}\right|_V \leq 0 \quad \left.\frac{\partial^2 F}{\partial V^2}\right|_T \geq 0. \quad (5.56)$$

I.e. G is concave in both variables p and T . Due to $F = G - pV$, it follows that F is also concave in T , but convex in p .

5.2.1 Free energy for T and N fixed

Since $F > 0$ is convex in V and $\frac{\partial F}{\partial V} = -p < 0$, $F(V)$ is a left curving line that is always positive and it is strictly monotonically decreasing (slope zero would mean $p = 0$).

The Legendre transform of the free energy $F(V, T, N)$ (in the variable V) is the free enthalpy

$$\begin{aligned} G(p, T, N) &= F(V(p), T, N) + pV \\ &= F(V(p), T, N) - \left.\frac{\partial F}{\partial V}\right|_T V \end{aligned}$$

For $T > T_c$ the second derivative $\frac{\partial^2 F}{\partial V^2} = -\frac{\partial p}{\partial V}$ is greater than zero for all V . For $T < T_c$, however, there is an interval (V_α, V_β) in which the second derivative is zero and $F(V)$ is a linear function in V . Hence,

$$\left. \frac{\partial F}{\partial V} \right|_T = -p = \text{const} = -p_{\alpha\beta}.$$

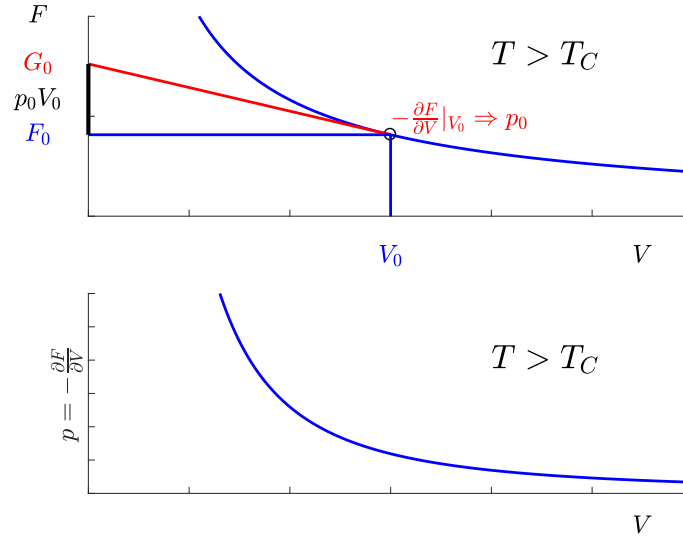


Figure 5.3: **Schematic plot of free energy for $T > T_c$.**

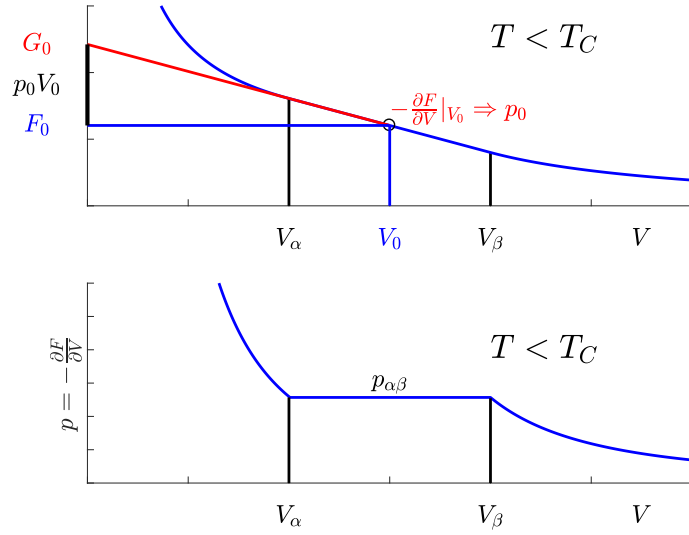
5.2.2 F and G as function of T

As function of temperature, both F and G behave similarly, since

$$-S = \left. \frac{\partial G}{\partial T} \right|_p = \left. \frac{\partial F}{\partial T} \right|_V.$$

At a first order phase transition the entropy S shows a finite jump at T_c , which is then associated with

LATENT HEAT	
$\Delta Q = T_{\alpha\beta} \Delta S . \tag{5.57}$	

Figure 5.4: **Schematic plot of free energy for $T < T_c$.**

ΔQ is, however not a material constant, it also depends on the state variables. E.g. for the liquid-gas system, ΔQ depends on pressure. On approaching the critical point, ΔD vanishes. The definition of the order of the phase transition has to be refined

5.2.3 Ehrenfest classification

N-TH ORDER PHASE TRANSITION			
<hr/>			
$\left. \frac{\partial^m G_\alpha}{\partial T^m} \right _p = \left. \frac{\partial^m G_\beta}{\partial T^m} \right _p$	$\forall m = 1, \dots, n-1,$	(5.58a)	
$\left. \frac{\partial^m G_\alpha}{\partial p^m} \right _T = \left. \frac{\partial^m G_\beta}{\partial p^m} \right _T$	$\forall m = 1, \dots, n-1.$	(5.58b)	
But			
$\left. \frac{\partial^n G_\alpha}{\partial T^n} \right _p \neq \left. \frac{\partial^n G_\beta}{\partial T^n} \right _p$		(5.58c)	
$\left. \frac{\partial^n G_\alpha}{\partial p^n} \right _T \neq \left. \frac{\partial^n G_\beta}{\partial p^n} \right _T.$		(5.58d)	

Of practical importance are first and second order phase transitions. First order phase transitions have already been discussed in detail. In the case of a second order phase transition, we have

SECOND ORDER PHASE TRANSITION			
<hr/>			
$G(T, p)$	continuous	(5.59a)	
$\left. \frac{\partial G}{\partial T} \right _p, \left. \frac{\partial G}{\partial p} \right _T, (\text{i.e. } S(T, p), V(T, p))$	continuous	(5.59b)	
$C_p = -T \left. \frac{\partial^2 G}{\partial T^2} \right _p \quad \kappa_T = -\frac{1}{V} \left. \frac{\partial^2 G}{\partial p^2} \right _T$	discontinuous	(5.59c)	

5.3 Critical exponents

Second order phase transitions are of particular interest, as they exhibit universal behaviour close to the phase transition. Completely different systems with second order phase transition show a very similar power law behaviour, which shall be discussed in this section. We define

$$\varepsilon = \frac{T - T_C}{T_C}$$

Very often it is observed that in a close vicinity of T_c , typically $|\varepsilon| < 10^{-2}$, physical observables $f(T)$ show the following behaviour

$$f(\varepsilon) = a\varepsilon^\varphi(1 + b\varepsilon^\psi + \dots) \quad \psi > 0 ,$$

here φ and ψ are real valued exponents. This behaviour is abbreviated as

$$f(\varepsilon) \simeq \varepsilon^\varphi , \quad (5.60)$$

One says: f behaves like ε^φ and φ is called the *critical exponent*. The critical exponent is more generally defined by

$$\varphi = \lim_{\varepsilon \rightarrow 0} \frac{\ln |f(\varepsilon)|}{\ln |\varepsilon|} \quad (5.61)$$

In general, the critical exponent depends on whether we compute it below or above T_c . For the order parameter it actually makes only sense below T_c , as the order parameter by definition is zero above T_c .

Of course, different observables may have different critical exponents. The critical observable for one observable, however, is almost universal, it only depends on

- spatial dimension
- range of the interaction
- spin dimensionality.

This is the so-called *universality hypothesis* of Griffiths. The range of the particle interaction is grouped into three classes:

- short-range, if the interaction decreases like

$$r^{-(d+2+\alpha)} ; \quad 0 < \alpha .$$

Where the details of the interaction are unimportant. One finds a really universal behaviour.

- long-range, if

$$r^{-(d+2+\alpha)} ; \quad \alpha < \frac{d}{2} - 2 \quad (\text{always negative}).$$

In this case, the *classical theories* apply (Landau Theory, van der Waals model, Weißferromagnet). In this case, however, the critical exponents are independent of the spatial dimension.

- Intermediate range, if

$$r^{-(d+2+\alpha)} ; \quad \frac{d}{2} - 2 < \alpha < 0 .$$

The critical exponents depend on α

Magnetic systems are typically discussed as interacting spin-systems. As spin-dimension (n) we understand the relevant components of the spin vector. Ising model /Potts model has $n = 1$ and is considered as one-dimensional vector, the $x - y$ -model has $n = 2$ and the vectors are two-dimensional, and finally the Heisenberg model $n = 3$ is three-dimensional. The critical exponents.

Possible behaviour:

Power law decay $f(\varepsilon) \simeq \varepsilon^\varphi$ with $\varphi > 0$

Power law divergence $f(\varepsilon) \simeq \varepsilon^\varphi$ with $\varphi < 0$

logarithmic divergence $f(\varepsilon) = a + b \ln(|\varepsilon|)$ we obtain by the definition of the critical exponent in equation (5.61) [\[previous page\]](#) $\varphi = 0$

In general, the critical exponent for $\varepsilon > 0$ (denoted by φ) can differ from that for $\varepsilon < 0$ (denoted by φ')

5.3.1 Important critical exponents

1. Heat capacity ($\alpha :_{\pm}$) for real gases

$$C_V \simeq A_{\pm} |\varepsilon|^{-\alpha_{\pm}} : \quad \begin{cases} - & \text{for path II, i.e. } T \nearrow T_c, \text{ with } \rho = \rho_{g,fl} \\ + & \text{for path I, i.e. } T \searrow T_c, \text{ with } \rho = \rho_c \end{cases} . \quad (5.62)$$

Heat capacity (α', α) for magnets

$$C_B \simeq A_{\pm} |\varepsilon|^{-\alpha_{\pm}} : \quad \begin{cases} - & T \nearrow T_c, \text{ with } B = 0 \\ + & \text{for path I, i.e. } T \searrow T_c, \text{ with } B = 0 \end{cases} . \quad (5.63)$$

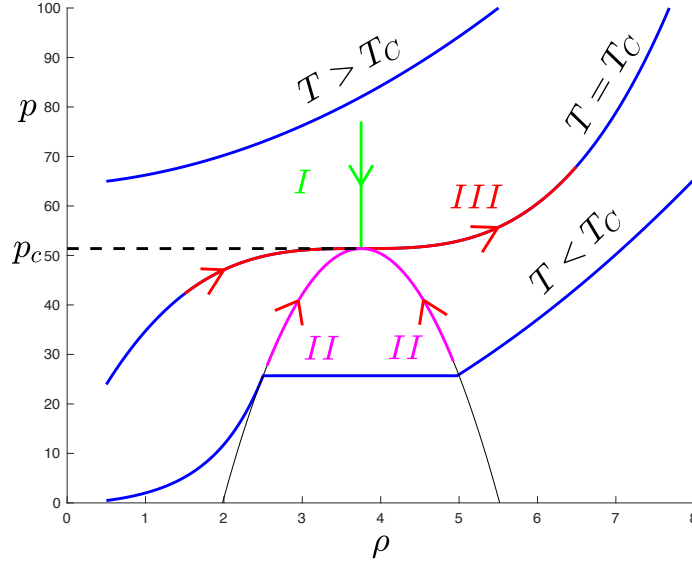


Figure 5.5: **Paths for the definition of the critical exponents.**

The experiment yields $\alpha_{\pm} \approx 0$. Ising 2D, exact solution, logarithmic divergence, i.e. $\alpha_{\pm} = 0$. Classic theories (i.e. Weißferro-magnet, vdW gas) yield discontinuity, which is equivalent to $\alpha_{\pm} = 0$.

2. Order parameter (β [not inverse temperature!]). A variable that exists only below T_c and which characterises the order of the system. E.g. magnetization M or the for real gases the density difference $\Delta\rho = \rho_{fl} - \rho_g$, or rather $\Delta\rho = \rho_{fl,g} - \rho_c$, in the two-phase region

$$\frac{\Delta\rho(T)}{2\rho_c} \simeq B|\varepsilon|^{\beta}, \text{ along path II} \quad (5.64)$$

$$\frac{M(T)}{M(0)} \simeq B|\varepsilon|^{\beta}, \text{ for } B = 0. \quad (5.65)$$

The normalizations are introduced to make sure that B is $O(1)$. In principle, β should be β' , as we are below T_c , but since the order parameter is only defined below T_c , it is common to use β . Typical experimental values are 0.35 ± 0.02 . classical theories yield $\beta = 1/2$. 2D Ising exact, $\beta = 1/8$. For the 3D Ising model one finds $\beta = 0.325 \pm 0.001$. While 3D Heisenberg gives $\beta = 0.3445 \pm 0.002$.

3. Compressibilities and susceptibilities (γ_{\pm})

$$\kappa_T = -\frac{1}{V} \frac{\partial V}{\partial p} \Big|_T = \frac{1}{\rho} \frac{\partial \rho}{\partial p} \Big|_T ,$$

$$\chi_T = \frac{\partial M}{\partial B} \Big|_T$$

$$\frac{\kappa_T}{\kappa_{T_c}^0} \simeq C_{\pm} |\varepsilon|^{\gamma_{\pm}} : \quad \begin{cases} - & \text{for path II, i.e. } T \nearrow T_c, \text{ with } \rho = \rho_{g,fl} \\ + & \text{for path I, i.e. } T \searrow T_c, \text{ with } \rho = \rho_c \end{cases} . \quad (5.66)$$

Here κ_c^0 is the compressibility of the ideal gas at $T = T_c$, which follows (due to $\rho = \frac{p}{k_B T}$) from

$$\kappa = \frac{1}{\rho} \frac{1}{k_B T} = \frac{1}{p} .$$

Similarly, one uses for the normalization in the magnetic case, the result of an ideal paramagnet

$$M = \frac{C^*}{T} ,$$

with C^* being the Curie constant.

$$\frac{\chi_T}{\chi_{T_c}^0} \simeq C_{\pm} |\varepsilon|^{-\gamma_{\pm}} : \quad \begin{cases} - & \text{for path II, i.e. } T \nearrow T_c, \text{ with } H = 0 \\ + & \text{for path I, i.e. } T \searrow T_c, \text{ with } H = 0 \end{cases} . \quad (5.67)$$

Typical experimental values differ somewhat about $\gamma \approx \gamma' \approx 1.3$. Model calculations all yield $\gamma = \gamma'$. Classical models $\gamma = 1$, 2D Ising exact, $\gamma = 7/4$, 3D Ising $\gamma \approx 1.24$, 3d Heisenberg $\gamma = 1.39$.

4. Critical isotherm (δ) We define the critical pressure of the ideal gas as the pressure of the ideal gas at T_c and ρ_c via the ideal gas law

$$p_c^{(0)} = k_B T_c \rho_c$$

which clearly differs from the relation of the vdW model (see equation (5.35) [p. 114]). For the real gas we define the isothermal critical exponent as

$$\frac{p - p_c}{p_c^0} \simeq D \left| \frac{\rho - \rho_c}{\rho_c} \right|^{\delta} \text{sign}(\rho - \rho_c) ; \quad (\text{along the path III, } T = T_c) . \quad (5.68)$$

If we define

$$B_C^{(0)} = \frac{k_B T_c}{\mu_0 m} m$$

with m being the magnetic moment per particle, then the corresponding relation for magnets reads

$$\frac{B}{B_C^{(0)}} \simeq D \left| \frac{M(T = T_c, B)}{M(T = 0, B = 0)} \right|^\delta \text{sign}(M) .$$

Experimental values are in the range $\delta \in (4, 5)$. The 2D Ising model yields $\delta = 15$, which far off. The 3D Ising and Heisenberg model yields $\delta = 4.9$ (much better). Classical theories yield $\delta = 3$.

5. Correlation lengths (ν, ν', η)

We define a pair-correlation function, e.g. density-density or spin-spin,

$$g(\mathbf{r}, \mathbf{r}') = \langle \Delta \rho(\mathbf{r}) \Delta \rho(\mathbf{r}') \rangle \quad (5.69)$$

$$g_{ij} = \langle \Delta \mathbf{S}_i \Delta \mathbf{S}_j \rangle . \quad (5.70)$$

In the critical regions they behave approximately like

ORNSTEIN-ZERNIKE FUNCTION

$$g(\mathbf{r}, \mathbf{r}') = c_0 \frac{e^{-\frac{|\mathbf{r}-\mathbf{r}'|}{\xi(T)}}}{|\mathbf{r} - \mathbf{r}'|} \quad (5.71)$$

$$g_{ij} = g(\mathbf{r}_i, \mathbf{r}_j) , \quad (5.72)$$

with $\xi(T)$ is the correlation length. It diverges on approaching the critical point. For real gases one defines

$$\xi \simeq D_\pm |\varepsilon|^{-\nu_\pm} : \quad \begin{cases} - & \text{on path II} , \\ + & \text{on path I} . \end{cases} \quad (5.73)$$

For magnets

$$\xi \simeq D_\pm |\varepsilon|^{-\nu_\pm} : \quad \begin{cases} - & \text{for } T \nearrow T > T_C, B = 0 , \\ + & \text{for } T \searrow T > T_C, B = 0 . \end{cases} \quad (5.74)$$

Finally, we also introduce the pair-correlation function at the critical temperature $T = T_c$. According to the Ornstein-Zernike formula in equation (5.71), at $T = T_c$ the correlation length is infinite and, therefore, the pair-correlation would decrease like $1/|\mathbf{r}-\mathbf{r}'|$. This is, however, not the case for real systems. The behaviour is slightly different and expressed by

$$g(\mathbf{r}, \mathbf{r}') = |\mathbf{r} - \mathbf{r}'|^{-(d-2+\eta)} \begin{cases} p = p_C & , \text{ real gases } , \\ B = 0, \text{ magnets } . \end{cases}$$

The Ornstein-Zernike formula would imply $\eta = 3 - d$. For the other critical exponents ν, ν' the deviation from the $1/r$ dependence is negligible, as the correlation length is obtained from the slope of a fit of

$$\ln(g(r)) = c_0 - \frac{r}{\xi(T)} - (d - 2 + \eta) \ln(r)$$

versus r . Here the last term enters only logarithmically in r .

5.3.2 Scaling laws

Generalized homogeneous functions $f(x, y, \dots)$ in several variables have the following property for arbitrary real λ

$$f(\lambda^{a_x} x, \lambda^{a_y} y, \dots) = \lambda f(x, y, \dots) , \quad (5.75)$$

where a_x, a_y, \dots can be any real numbers. An example would be

$$f(x, y) = 4x^3 + 7y^8 ,$$

with $a_x = 1/3$ and $a_y = 1/8$, while

$$f(x, y) = x + 6x^2 + xy + y^5$$

is no generalized homogeneous function. Next we will define the scaling hypothesis in the case of the free energy $F(T, B)$ of a magnetic system. We are only interested in the non-analytic parts of F near T_C which we denote by $F(\varepsilon, B)$.

SCALING HYPOTHESIS
<div style="text-align: right; margin-right: 20px;"> $F(\lambda^{a_\varepsilon} \varepsilon, \lambda^{a_B} B) = \lambda F(\varepsilon, B) . \quad (5.76)$ </div>

This is not yet strictly proven in general, but there are many important cases where the scaling hypothesis is fulfilled.

Now we can use the scaling hypothesis to express the critical exponents in terms of the scaling parameters a_ε and a_B . Differentiation w.r.t. B yields

$$\lambda^{a_B} \frac{\partial}{\partial \lambda^{a_B} B} F(\lambda^{a_\varepsilon} \varepsilon, \lambda^{a_B} B) = \lambda \frac{\partial}{\partial B} F(\varepsilon, B) .$$

Now we have

$$M = -\frac{\partial F}{\partial B}$$

and therefore we have

$$\lambda^{a_B} M(\lambda^{a_\varepsilon} \varepsilon, \lambda^{a_B} B) = \lambda M(\varepsilon, B) . \quad (5.77)$$

1. Exponent β . We use $B = 0$ and obtain

$$M(\lambda^{a_\varepsilon} \varepsilon, 0) = \lambda M(\varepsilon, 0) ,$$

which is valid for any λ , also for

$$\lambda = (-\varepsilon)^{-1/a_\varepsilon} ,$$

resulting in

$$M(\varepsilon, 0) = (-\varepsilon)^{\frac{1-a_B}{a_\varepsilon}} M(-1, 0) \simeq (-\varepsilon)^{\frac{1-a_B}{a_\varepsilon}} .$$

Hence,

$$\beta = \frac{1 - a_B}{a_\varepsilon} .$$

2. Exponent δ (critical isotherm) Next we use $\varepsilon = 0$ and have

$$M(0, B) = \lambda^{a_B-1} M(0, \lambda^{a_B} B) .$$

Here we choose $\lambda = B^{-1/a_B}$ and obtain

$$M(0, B) \simeq B^{\frac{1-a_B}{a_B}}$$

$$B \simeq M^{\frac{a_B}{1-a_B}} ,$$

and hence $\delta = \frac{a_B}{1-a_B}$. In summar, we have

$$a_B = \frac{\delta}{1 + \delta} \quad (5.78)$$

$$a_\varepsilon = \frac{1}{\beta} \frac{1}{1 + \delta} \quad (5.79)$$

$$(5.80)$$

We can express further critical exponents in terms of the scaling parameters, which then in turn allows to find relations among the critical exponents: From the scaling laws one finds

$$\alpha = \alpha' ; \quad \gamma = \gamma' ; \quad \nu = \nu' . \quad (5.81)$$

and also

$$\alpha + 2\beta + \gamma = 2 \quad (5.82)$$

$$\alpha + \beta(1 + \delta) = 2 \quad (5.83)$$

$$\beta = \frac{\gamma}{\delta - 1} \quad (5.84)$$

$$\nu = \frac{\gamma}{2 - \eta} . \quad (5.85)$$

5.3.3 Pottsmodel

It can be considered as generalisation of the Ising model, where the spin can take on more than just two values. Usually they are enumerated $s \in \{1, 2, \dots, q\}$. It is called the *q-state Potts model*. The Hamiltonian of the Potts model reads

<p>POTTSMODEL (<i>q states</i>)</p> <hr style="border: 0.5px solid black;"/> $H_P = -J \sum_{ij} \delta_{s_i s_j} , \quad (5.86)$

i.e. when spins on neighbouring sites are equal, they experience a lower energy ($E = -J$) than when they have different spin values ($E = 0$). The Potts model is used to study the behaviour of ferromagnets and other phenomena of solid-state physics.

Apart from statistical physics it is also used in computer science (signal processing) and biology (neural networks).

The strength of the Potts model is not so much that it models these physical systems well; it is rather that the one-dimensional case is exactly solvable, and that it has interesting physical properties. For $d \geq 2$ it shows a phase transition. It is second order for $q \leq 4$ and first order for $q > 4$.

5.3.4 Maxwell Relations

We know

$$dU(S, V, N) = TdS - pdV + \mu dN$$

Hence

$$\begin{aligned} \left. \frac{\partial U(S, V, N)}{\partial S} \right|_{V, N} &= T(S, V, N) \\ \left. \frac{\partial U(S, V, N)}{\partial V} \right|_{S, N} &= -p(S, V, N) . \end{aligned}$$

From this we obtain

$$\left. \frac{\partial T}{\partial V} \right|_{S, N} = \frac{\partial}{\partial V} \left(\left. \frac{\partial U}{\partial S} \right|_{V, N} \right) \Big|_{S, N} = \frac{\partial}{\partial S} \left(\left. \frac{\partial U}{\partial V} \right|_{S, N} \right) \Big|_{V, N} = - \left. \frac{\partial p}{\partial S} \right|_{V, N}$$

In the following we use the convention

$$\frac{\partial^2 f(x, y, z)}{\partial x \partial y} = \frac{\partial}{\partial y} \left(\left. \frac{\partial f}{\partial x} \right|_{y, z} \right) \Big|_{x, z} .$$

and we can simplify the former equation to

$$\left. \frac{\partial T}{\partial V} \right|_{S, N} = - \left. \frac{\partial p}{\partial S} \right|_{V, N} = \frac{\partial^2 U(S, V, N)}{\partial S \partial V} .$$

Similarly we find with

$$\begin{aligned} \left. \frac{\partial F(T, V, N)}{\partial T} \right|_{V, N} &= -S(T, V, N) \\ \left. \frac{\partial F(T, V, N)}{\partial V} \right|_{S, N} &= -p(T, V, N) . \end{aligned}$$

the relation

$$\left. \frac{\partial S(T, V, N)}{\partial V} \right|_{T, N} = \left. \frac{\partial p(T, V, N)}{\partial T} \right|_{V, N} = - \frac{\partial^2 F(T, V, N)}{\partial V \partial T}$$

Based on the free enthalpy $G(T, p, N)$ we obtain with

$$\begin{aligned} \left. \frac{\partial G(T, p, N)}{\partial T} \right|_{p, N} &= -S(T, p, N) \\ \left. \frac{\partial G(T, p, N)}{\partial p} \right|_{S, N} &= V(T, p, N) . \end{aligned}$$

the relation

$$-\left.\frac{\partial S(T, p, N)}{\partial p}\right|_{T, N} = \left.\frac{\partial V(T, p, N)}{\partial T}\right|_{p, N} = \frac{\partial^2 G(T, p, N)}{\partial p \partial T}$$

Finally, we introduce the *enthalpy* $H(S, p, N)$ via the Legendre transformation of $U(S, V, N)$ with respect to V , i.e.

$$H(S, p, N) = U(S, V, N) + pV ,$$

for which we have

$$\begin{aligned} \left.\frac{\partial H(S, p, N)}{\partial S}\right|_{p, N} &= T(S, p, N) \\ \left.\frac{\partial H(S, p, N)}{\partial p}\right|_{S, N} &= V(S, p, N) . \end{aligned}$$

Then we find

$$\left.\frac{\partial T(S, p, N)}{\partial p}\right|_{S, N} = \left.\frac{\partial V(S, p, N)}{\partial S}\right|_{p, N} = \frac{\partial^2 H(S, p, N)}{\partial p \partial S}$$

We summaries these results

MAXWELLRELATIONS			
$\left.\frac{\partial T(S, V, N)}{\partial V}\right _{S, N}$	$= -\left.\frac{\partial p(S, V, N)}{\partial S}\right _{V, N}$	$= \frac{\partial^2 U(S, V, N)}{\partial S \partial V}$	(5.87a)
$\left.\frac{\partial S(T, V, N)}{\partial V}\right _{T, N}$	$= \left.\frac{\partial p(T, V, N)}{\partial T}\right _{V, N}$	$= -\frac{\partial^2 F(T, V, N)}{\partial V \partial T}$	(5.87b)
$-\left.\frac{\partial S(T, p, N)}{\partial p}\right _{T, N}$	$= \left.\frac{\partial V(T, p, N)}{\partial T}\right _{p, N}$	$= \frac{\partial^2 G(T, p, N)}{\partial p \partial T}$	(5.87c)
$\left.\frac{\partial T(S, p, N)}{\partial p}\right _{S, N}$	$= \left.\frac{\partial V(S, p, N)}{\partial S}\right _{p, N}$	$= \frac{\partial^2 H(S, p, N)}{\partial p \partial S}$	(5.87d)

5.3.5 Ehrenfest equations

Next we derive the analogue of Clausius-Clapeyron for second order phase transitions. In this case, S and V are continuous when crossing the phase

boundary. Along a phase boundary between phase α and β we therefore have in the Gibbs ensemble (T, p, N) fixed

$$\begin{aligned} S_\alpha(T, p, N) &= S_\beta(T, p, N) \\ V_\alpha(T, p, N) &= V_\beta(T, p, N) , \end{aligned}$$

and also

$$\begin{aligned} dS_\alpha &= dS_\beta \\ dV_\alpha &= dV_\beta . \end{aligned}$$

We can use these equations, to obtain dp/dT along the phase boundary. We combine these equation as

$$dX_\alpha(T, p, N) = dX_\beta(T, p, N) ,$$

where X stands either for S or V . Since N is fixed, it will not vary along the phase boundary. We therefore have

$$\left. \frac{\partial X_\alpha}{\partial T} \right|_{p,N} dT + \left. \frac{\partial X_\alpha}{\partial p} \right|_{T,N} dp = \left. \frac{\partial X_\beta}{\partial T} \right|_{p,N} dT + \left. \frac{\partial X_\beta}{\partial p} \right|_{T,N} dp ,$$

from which we obtain

$$\begin{aligned} \left(\left. \frac{\partial X_\beta}{\partial T} \right|_{p,N} - \left. \frac{\partial X_\alpha}{\partial T} \right|_{p,N} \right) dT &= - \left(\left. \frac{\partial X_\beta}{\partial p} \right|_{T,N} - \left. \frac{\partial X_\alpha}{\partial p} \right|_{T,N} \right) dp \\ \frac{dp}{dT} &= - \frac{\left. \frac{\partial X_\beta}{\partial T} \right|_{p,N} - \left. \frac{\partial X_\alpha}{\partial T} \right|_{p,N}}{\left. \frac{\partial X_\beta}{\partial p} \right|_{T,N} - \left. \frac{\partial X_\alpha}{\partial p} \right|_{T,N}} := - \frac{\Delta \left. \frac{\partial X_\beta}{\partial T} \right|_{p,N}}{\left. \frac{\partial \Delta X_\beta}{\partial p} \right|_{T,N}} \end{aligned}$$

If we insert S for X we find

$$\frac{dp}{dT} = - \frac{\Delta \left. \frac{\partial S}{\partial T} \right|_{p,N}}{\left. \frac{\partial \Delta S}{\partial p} \right|_{T,N}} . \quad (5.88)$$

We use

$$\left. \frac{\partial S}{\partial T} \right|_{p,N} = \frac{1}{T} C_p ,$$

and from the Maxwell relations we use

$$\left. \frac{\partial S}{\partial p} \right|_{T,N} = - \left. \frac{\partial V}{\partial T} \right|_{p,N} .$$

The change in volume w.r.t. temperature is related to the α

COEFFICIENT OF THERMAL EXPANSION <i>(for constant pressure)</i>	
$\alpha_p := \frac{1}{V} \left. \frac{\partial V}{\partial T} \right _{p,N}$	(5.89)

With these response functions, we find

$$\left. \frac{dp}{dT} \right|_{\text{ph.b.}} = \frac{1}{VT} \frac{\Delta C_p}{\Delta \alpha_p} . \quad (5.90)$$

Alternatively, if we use V as X , we have

$$\frac{dp}{dT} = - \frac{\left. \Delta \frac{\partial V}{\partial T} \right|_{p,N}}{\left. \frac{\partial \Delta V}{\partial p} \right|_{T,N}} . \quad (5.91)$$

Here we employ the relations

$$\begin{aligned} \alpha_p &= \frac{1}{V} \left. \frac{\partial V}{\partial T} \right|_{p,N} \\ \kappa_p &= - \frac{1}{V} \left. \frac{\partial V}{\partial p} \right|_{T,N} , \end{aligned}$$

and find

$$\left. \frac{dp}{dT} \right|_{\text{ph.b.}} = \frac{\Delta \alpha_p}{\Delta \kappa_p} . \quad (5.92)$$

In summary we have the

EHRENFEST EQUATIONS

$$\left. \frac{dp}{dT} \right|_{\text{ph.b.}} = \frac{\Delta\alpha_p}{\Delta\kappa_p} = \frac{1}{VT} \frac{\Delta C_p}{\Delta\alpha_p} . \quad (5.93)$$

5.4 Ising again

$$s := \sinh(2K)$$

$$f = \frac{F}{JN} = -K \left[\frac{\ln(2)}{2} + \frac{1}{4\pi} \int_0^{2\pi} \log \left(1 + s^4 + \sqrt{1 + s^4 - 2s^2 \cos(x)} \right) dx \right]$$

T_c from

$$s_c = \sinh(2K_c) = 1$$

$$K_c = J\beta_c = 0.440687$$

$$\frac{k_B T_c}{J} = 2.26919 .$$

$$u = \frac{U}{JN} = -\coth(2K) \left[1 + \frac{2(2 \tanh^2(2K) - 1)}{\pi} \int_0^{\pi/2} \frac{1}{\sqrt{1 - \frac{4k}{(1+k)^2} \sin^2(x)}} dx \right]$$

For $T \leq T_c$

$$M(T) = \left[1 - \left(\sinh^{-4}(2K) \right) \right]^{1/8} .$$

$$S = -\frac{\partial F}{\partial T} = -\frac{\partial F}{\partial \beta} \frac{d\beta}{dT} = \frac{J}{k_B T^2} \frac{\partial F}{\partial J\beta}$$

$$= \frac{K}{T} \frac{\partial F}{\partial K} = \frac{K J N}{T} \frac{\partial f}{\partial K}$$

$$\frac{S}{N} = k_B \frac{K J}{k_B T} \frac{\partial f}{\partial K}$$

$$s = \frac{S}{k_B N} = K^2 \frac{\partial f}{\partial K}$$

$$\begin{aligned}
U &= F + TS = fJN + Ts k_B N \\
&= JN \left(f + \frac{T k_B}{J} s \right) \\
u &= f + \frac{s}{K}
\end{aligned}$$

$$\begin{aligned}
s &= Kf - K^3 \frac{d}{dK} \frac{1}{4\pi} \int_0^{2\pi} \log \left(1 + s^2 + \sqrt{1 + s^4 - 2s^2 \cos(x)} \right) dx \\
&= Kf - K^3 \left(\frac{d}{ds} \frac{1}{4\pi} \int_0^{2\pi} \log \left(1 + s^2 + \sqrt{1 + s^4 - 2s^2 \cos(x)} \right) dx \right) \frac{d}{dK} \sinh(2K) \\
&= K \left(f - K^2 \left(\frac{d}{ds} \frac{1}{4\pi} \int_0^{2\pi} \log \left(1 + s^2 + \sqrt{1 + s^4 - 2s^2 \cos(x)} \right) dx \right) 2\sqrt{1 + s^2} \right).
\end{aligned}$$

$$u = f + \frac{s}{K}$$

Chapter 6

Magnetism

6.1 Hamiltonian

The hamiltonian reads

$$H = \sum_j \left(\mathbf{p}_j + e\mathbf{A}(\mathbf{r}_j) \right)^2 + H_{\text{Coul}} - \sum_j m_j^s B(\mathbf{r}_j) + H_{\text{rel}} \quad (6.1)$$

So far, this hamiltonian describes any arbitrary system, from isolated atoms up to any crystal. The first term describes the coupling of the electrons to the electromagnetic field in combination with the kinetic energy of the electrons, the second contains Coulomb interaction of the electrons to the atomic core and the electron-electron interaction and last term covers the interaction of the magnetic moment of the electronic spins to the external field. The spin of electron j , denoted by \mathbf{S}_j corresponds to a magnetic moment

$$\mathbf{m}_j^s = -\frac{g_e e}{2m} \mathbf{S}_j = -\frac{g_e \mu_B}{\hbar} \mathbf{S}_j \quad (6.2)$$

with $g_e = 2.0023$ being the Landé Factor for the electron, and the Bohr magneton

$$\mu_B = \frac{e\hbar}{2m}. \quad (6.3)$$

The last term in equation (6.1) covers relativistic effects, such as the spin orbit coupling, which we will briefly discuss later on. In the hamiltonian the dipol-dipol interaction of the spins is neglected, as is of minor importance. First, we transform the first part of the hamiltonian

$$\left(\mathbf{p}_j + e\mathbf{A}(\mathbf{r}_j) \right)^2 = \mathbf{p}_j^2 + e\mathbf{p}_j \mathbf{A}(\mathbf{r}_j) + e\mathbf{A}(\mathbf{r}_j) \mathbf{p}_j + e^2 \mathbf{A}^2(\mathbf{r}_j)$$

We use the Coulomb gauge, in which

$$\operatorname{div} \mathbf{A}(\mathbf{r}) = 0$$

holds. Moreover, we will only consider a homogeneous magnetic field \mathbf{B} , for which in the Coulomb gauge we can write

$$\mathbf{A}(\mathbf{r}) = \frac{1}{2} \mathbf{B} \times \mathbf{r} .$$

In this case

$$\mathbf{p}_j \mathbf{A}(\mathbf{r}_j) = \frac{1}{2} \mathbf{p}_j \cdot (\mathbf{B} \times \mathbf{r}_j) .$$

We have to take into account that \mathbf{P} and \mathbf{r} are operators, while \mathbf{B} is a classical vector. Then the spin-term simplifies to

$$\sum_j m_j^s B(\mathbf{r}_j) = \mathbf{B} \cdot \sum_j m_j^s .$$

Moreover, we need

$$\begin{aligned} \mathbf{p} \cdot (\mathbf{B} \times \mathbf{r}) &= p_i \varepsilon_{ijk} B_j r_k \\ &= -B_j \varepsilon_{jik} p_i r_k \\ &= B_j \varepsilon_{jki} r_k p_i . \end{aligned}$$

IN the last step we have used that r_k and p_j commute for different indices, which is guaranteed by the Levi Civita tensor. Hence

$$\mathbf{p}_j \cdot (\mathbf{B} \times \mathbf{r}_j) = \mathbf{B} \cdot (\mathbf{r}_j \times \mathbf{p}_j) = \mathbf{B} \cdot \mathbf{L}_j . \quad (6.4)$$

Similarly, we find

$$\begin{aligned} (\mathbf{B} \times \mathbf{r}) \cdot \mathbf{p} &= \varepsilon_{ijk} B_j r_k p_i \\ &= B_j \varepsilon_{jki} r_k p_i . \end{aligned}$$

We still need

$$\begin{aligned} \mathbf{A}^2(r) &= \frac{1}{4} \left(\mathbf{B} \times \mathbf{r} \right)^2 \\ &= \frac{1}{4} \varepsilon_{ijk} \varepsilon_{imn} B_i r_j B_m r_n \\ &= \frac{1}{4} \left(B_i r_j B_i r_j - B_i r_i B_j r_j \right) \\ &= \frac{1}{4} (\mathbf{B}^2 \mathbf{r}^2 - (\mathbf{B} \cdot \mathbf{r})^2) . \end{aligned}$$

In total we therefore find

$$H = \frac{1}{2m} \sum_j \mathbf{p}_j^2 + \frac{e}{2m} \mathbf{B} \sum_j \cdot \mathbf{L}_j + \frac{e^2 B^2}{8m} \sum_j (\mathbf{B}^2 \mathbf{r}_j^2 - (\mathbf{B} \cdot \mathbf{r}_j)^2) + H_{\text{Coul}} - \mathbf{m}^s \cdot \mathbf{B} ,$$

where \mathbf{m}^s is the total magnetic moment of all spins. We also relate the angular momentum with the magnetic moment

$$\begin{aligned} \mathbf{m}_j^L &= -\frac{e}{2m} \mathbf{L}_j = -\frac{\mu_B}{\hbar} \mathbf{L}_j \\ \mathbf{m}^L &= -\frac{e}{2m} \sum_j \mathbf{L}_j = -\frac{\mu_B}{\hbar} \sum_j \mathbf{L}_j . \end{aligned}$$

Then the hamiltonian simplifies to

$$\begin{aligned} H &= \frac{1}{2m} \sum_j \mathbf{p}_j^2 + H_{dia} + H_{\text{Coul}} - \mathbf{m}^{perm} \cdot \mathbf{B} , \\ H_{dia} &= \frac{e^2 B^2}{8m} \sum_j (\mathbf{B}^2 \mathbf{r}_j^2 - (\mathbf{B} \cdot \mathbf{r}_j)^2) , \end{aligned}$$

with the total *permanent* magnetic moment defined by

$$\mathbf{m}^{perm} = \mathbf{m}^s + \mathbf{m}^L = -\frac{\mu_B}{\hbar} (\mathbf{L} + g_e \mathbf{S}) . \quad (6.5)$$

It results in *paramagnetism*.

The permanent moments tend to align in the magnetic field, while thermal fluctuations have the opposite effect. There is yet another term in the hamiltonian equation (6.1) [p. 137] that contains magnetic moments resulting from the electronic motion: the diamagnetic term H_{dia} . One can show that the total magnetic moment, defined as

$$\mathbf{m} = \mathbf{m}^{perm} + \mathbf{m}^{ind} ,$$

can be obtained by

$$\mathbf{m} = -\nabla_{\mathbf{B}} H .$$

Then we see that the induced magnetic moment is given by

$$\mathbf{m}^{ind} = -\frac{e^2}{4m} \sum_j (\mathbf{r}_j^2 \mathbb{1} - \mathbf{r}_j \mathbf{r}_j^T) \mathbf{B} .$$

W.l.o.g. we can choose $\mathbf{B} = B \mathbf{e}_z$ then

$$\mathbf{m}^{ind} = -B \frac{e^2}{4m} \sum_j (\mathbf{r}_j^2 \mathbf{e}_z - z_j \mathbf{r}_j)$$

6.1.1 Diamagnetism of atoms

We consider atoms or ions with closed shells, e.g. helium or other noble gases. in this case $S = 0$, $L = 0$. Then the only term contribution to a magnetic moment is the diamagnetic term. We will treat this term in first order perturbation theory, i.e. we first determine the ground state of the system for $B = 0$ and use the corresponding eigenvectors to determine the first order energy correction

$$\Delta E_1 = \langle H_{dia} \rangle ,$$

from which we obtain the resulting moment

$$\langle \mathbf{m}^{ind} \rangle = -B \frac{e^2}{4m} \sum_j (\langle \mathbf{r}_j^2 \rangle \mathbf{e}_z - \langle z_j \mathbf{r}_j \rangle) .$$

where $r_{j,\nu}$ is the ν -the cartesian component of the vector \mathbf{r}_j . We consider

$$\langle z_j \mathbf{r}_j \rangle = \sum_{\nu} \mathbf{e}_{\nu} \langle z_j r_{j,\nu} \rangle ,$$

For closed atomic shells, the ground state wavefunction is rotational invariant, therefore

$$\langle z_j r_{j,\nu} \rangle = \delta_{\nu,z} \langle z_j^2 \rangle = \delta_{\nu,z} \frac{1}{3} \langle r_j^2 \rangle$$

So in total , the atomic induced magnetic moment is

$$\mathbf{m}_{ind} = -\mathbf{B} \frac{e^2}{6m} \sum_j \langle r_j^2 \rangle$$

The magnetic moment is always in the opposite direction of the applied magnetic field, i.e. *diamagnetic reaction*, it reduced the total magnetic field. It is called *Langevin diamagnetism*.

From the magnetic moment, we determine the magnetic susceptibility

$$\chi_{\nu\mu} = \mu_0 \frac{\partial \langle \mathbf{m}_{\nu} \rangle}{\partial B_{\mu}} = -\delta_{\mu\nu} \frac{\mu_0 e^2}{6m} \langle \sum_j r_j^2 \rangle$$

To estimate the order of magnitude, we replace $\langle r_j^2 \rangle$ by the square of the Bohr radius. One obtains

$$\chi_{\text{per mole}} \approx -3 \times 10^{-6} \frac{\text{cm}^3}{\text{mol}} .$$

For noble gases this value is This diamagnetic contribution is also present in in open shell systems, but then it is orders of magnitude smaller than the contribution of the other term.

	He	Ne	Ar	Kr	Xe
χ per mole in $10^{-6}\text{cm}^3/\text{mole}$	-1.9	-7.2	-15.4	-28.0	-43.0

6.2 Density matrix and thermodynamic relations

We consider the canonical ensemble with fixed particle number N , which we will not explicitly mention as natural variable in the arguments. We only write T and \mathbf{B}

$$\rho(T, \mathbf{B}) = \frac{1}{Z(T, \mathbf{B})} e^{-\beta H}$$

$$Z = \text{tr} e^{-\beta H} .$$

The free energy reads

$$F(T, \mathbf{B}) = -k_B T \ln(Z(T, \mathbf{B})) . \quad (6.6)$$

The internal energy follows from

$$\begin{aligned} U &= \langle H \rangle = -\frac{\partial}{\partial \beta} \ln(Z) \\ &= \frac{\partial}{\partial \beta} (\beta F) \\ &= F - \underbrace{\beta(k_B T^2)}_{=T} \underbrace{\frac{\partial}{\partial T} F}_{=-S} \\ U &= F - TS . \end{aligned}$$

This is equivalent to

$$\begin{aligned} S &= \frac{1}{T} (U - F) \\ &= k_B \text{tr} \{ \rho(\beta H) \} + k_B \ln(Z) \\ &= k_B \left(\text{tr} \{ \rho(\beta H) \} + \ln(Z) \right) . \end{aligned}$$

Then we use

$$\begin{aligned} \ln(\rho) &= \ln \left(\frac{e^{-\beta H}}{Z} \right) = \ln \left(e^{-\beta H} \right) - \ln(Z) = -\beta H - \ln(Z) \\ \beta H &= - \left(\ln(\rho) + \ln(Z) \right) . \end{aligned}$$

Inserting above yields

$$\begin{aligned}
 S &= k_B \left(-\text{tr} \{ \rho (\ln(\rho) + \ln(Z)) \} + \ln(Z) \right) \\
 &= k_B \left(-\text{tr} \{ \rho \ln(\rho) \} - \underbrace{\text{tr} \{ \rho \} \ln(Z)}_{\substack{=1 \\ =0}} + \ln(Z) \right) \\
 &= \text{tr} \{ -k_B \rho \ln(\rho) \} \\
 &= -k_B \langle \ln(\rho) \rangle .
 \end{aligned}$$

Hence the entropy is the trace of the quantum entropy operator.
For the total differential of F we have

$$\begin{aligned}
 dF &= \left. \frac{\partial F(T, \mathbf{B})}{\partial T} \right|_{\mathbf{B}} dT + \left. \nabla_{\mathbf{B}} F(T, \mathbf{B}) \right|_T \cdot d\mathbf{B} \\
 &= -SdT - \mathbf{M} \cdot d\mathbf{B}
 \end{aligned}$$

Prove of the last step

$$\begin{aligned}
 \left. \nabla_{\mathbf{B}} F(T, \mathbf{B}) \right|_T &= -k_B T \nabla_{\mathbf{B}} \ln(Z) \\
 &= -\frac{k_B T}{Z} \nabla_{\mathbf{B}} Z \\
 &= -\frac{k_B T}{Z} \text{tr} \left(\left. \nabla_{\mathbf{B}} e^{-\beta H} \right|_T \right) \\
 &= \underbrace{-\frac{k_B T}{Z} (-\beta)}_{=\frac{1}{Z}} \text{tr} \left(e^{-\beta H} \underbrace{\left. \nabla_{\mathbf{B}} H \right|_T}_{=-\mathbf{m}} \right) \\
 &= -\text{tr} \left(\frac{e^{-\beta H}}{Z} \mathbf{m} \right) = -\mathbf{M}
 \end{aligned}$$

Hence

$$\left. \frac{\partial F}{\partial \mathbf{B}} \right|_T = -\mathbf{M} . \tag{6.7}$$

Oftentimes the magnetization is defined as total mean magnetic moment per volume.

6.2.1 Magnetic response functions

Specific heat in analogy to the case of gases

$$C_{\mathbf{B}} = \left. \frac{\partial U}{\partial T} \right|_{\mathbf{B}} = T \left. \frac{\partial S}{\partial T} \right|_{\mathbf{B}} = -T \left. \frac{\partial^2 F}{\partial T^2} \right|_{\mathbf{B}} . \tag{6.8}$$

Derivation as before without magnetic field.

Magnetic susceptibility

$$\chi_{T,\nu\mu} = \mu_0 \left. \frac{\partial M_\nu}{\partial B_\mu} \right|_T = -\mu_0 \frac{\partial^2 F}{\partial B_\nu \partial B_\mu} \quad (6.9)$$

In many times, the susceptibility is also expressed per volume.

6.2.2 Internal energy

We have defined the internal energy as $U = \langle H \rangle$, which is the energy of the material including the interaction of the electro magnetic field. It was derived from the purely electronic part. However, the field energy itself is not included. It is common to define a second internal energy U' that also includes the field energy

$$U' = U + \mathbf{M} \cdot \mathbf{B} . \quad (6.10)$$

resulting in

$$dU' = TdS + \mathbf{B} \cdot d\mathbf{M} .$$

It is the Legendre transformation in the pair (\mathbf{M}, \mathbf{B}) .

With

$$\begin{aligned} \left. \frac{\partial U'}{\partial S} \right|_{\mathbf{M}} &= T \\ \left. \frac{\partial U'}{\partial \mathbf{M}} \right|_S &= \mathbf{B} . \end{aligned}$$

It results in the Maxwell relation

$$\left. \frac{\partial \mathbf{B}}{\partial S} \right|_{\mathbf{M}} = \left. \frac{\partial T}{\partial \mathbf{M}} \right|_S .$$

6.3 Paramagnetism of independent moments

We consider the situation, where the permanent magnetic moments of the atoms do not interact. Then the hamiltonian has the structure

$$H = \sum_i H^{(i)} .$$

where i enumerates the atoms. All atoms shall be the same, so all $H^{(i)}$ are the same. In the following we suppress the index i . The hamiltonian $H^{(i)}$ has the form

$$H^{(i)} = H_0 + \underbrace{\gamma(\mathbf{LS})}_{\text{spin-orbit coupling}} + \underbrace{\frac{\mu_B B}{\hbar} (J^z + S^z)}_{\text{Zeeman term}}. \quad (6.11)$$

Here $J^z = L^z + S^z$. w.l.o.g. we have assumed that $\mathbf{B} = B\mathbf{e}_z$. In addition we have used $g_e \approx 2$.

H_0 commutes with L^2, S^2, L^z, S^z . Which is also true for the total hamiltonian without spin-orbit coupling. For the calculation of the partition function we have, since there is no interaction between the atoms

$$Z^N = (Z^1)^N,$$

i.e. it suffices to consider a single atom.

6.3.1 Weak spin-orbit coupling

In this case we ignore the spin-orbit term and the eigenvectors are given by

$$|\kappa, L, S, L_z, S_z\rangle,$$

where γ covers all other quantum numbers. The corresponding eigenvalues are based on equation (6.11) with J^z replaced by $L^z + S^z$.

$$E(\kappa, L, S, L_z, S_z) = E_0(\kappa, L, S) + \frac{\mu_B B}{\hbar} (L_z + 2S_z),$$

The canonical partition function reads

$$Z = \prod_{i=1}^N Z^{(i)} = \left(Z^{(1)} \right)^N \quad (6.12)$$

$$Z^{(1)} = \sum_{\kappa, L, S, L_z, S_z} e^{-\beta E_0(\kappa, L, S) - \frac{\beta \mu_B B}{\hbar} (L_z + 2S_z)} \quad (6.13)$$

$$Z^{(1)} = \sum_{\kappa, L, S} e^{-\beta E_0(\kappa, L, S)} \sum_{L_z, S_z} e^{-\frac{\beta \mu_B B}{\hbar} (L_z + 2S_z)}. \quad (6.14)$$

Typically, the Zeeman splitting is small compared to the other energy differences, when changing κ, L, S . For moderate temperature we only need to

consider the ground state quantum numbers (κ_0, L_0, S_0) (Hund's rule) and obtain (we use $L_z = \hbar l_z$ and $S_z = \hbar s_z$, with $l_z, s_z \in \mathbb{N}$)

$$Z^{(1)} = e^{-E_0(\kappa_0, L_0, S_0)} \underbrace{\sum_{l_z=-L_0}^{L_0} e^{-bL_z} \sum_{s_z=-S_0}^{S_0} e^{-2bs_z}}_{=Z(L_0, S_0)}$$

Here $b = \beta B \mu_B$. If there is a gap between the ground state multiplet and the first excited one of ΔE , then the next to leading order contribution $((\kappa_1, L_1, S_1))$ is

$$\begin{aligned} Z^{(1)} &= e^{-\beta E_0(\kappa_0, L_0, S_0)} Z(L_0, S_0) + e^{-E_0(\kappa_1, L_1, S_1)} Z(L_1, S_1) \\ &= e^{-\beta E_0(\kappa_0, L_0, S_0)} \left(Z(L_0, S_0) + e^{-\beta \Delta E} Z(L_1, S_1) \right) \end{aligned}$$

If $|\Delta E| \gg k_B T$ then we can neglect the higher order terms and

$$Z^{(1)} = e^{-\beta E_0(\kappa_0, L_0, S_0)} Z(L_0, S_0) \quad (6.15)$$

The key elements are sums of the form

$$\begin{aligned} z_M(\eta) &= \sum_{m=-M}^M e^{-\eta m} = e^{\eta M} \sum_{m=0}^{2M} e^{-\eta m} = e^{\eta M} \frac{1 - e^{-\eta(2M+1)}}{1 - e^{-\eta}} \\ &= \frac{e^{\eta(M+1/2)} - e^{-\eta(M+1/2)}}{e^{\eta/2} - e^{-\eta/2}} \\ &= \frac{\sinh(\eta(M+1/2))}{\sinh(\eta/2)} \end{aligned}$$

Then we obtain immediately

$$\begin{aligned} \frac{F}{N} &= -k_B T \ln(Z^1) \\ &= E_0(\kappa_0, L_0, S_0) - k_B T \ln \left(z_{L_0}(b) \right) - k_B T \ln \left(z_{S_0}(2b) \right). \end{aligned}$$

Next we compute the magnetisation

$$\mathbf{M} = - \frac{\partial F}{\partial \mathbf{B}} \Big|_T$$

Since $\mathbf{B} = \mathbf{e}_z$ we obtain

$$\mathbf{M} = -\mathbf{e}_z \frac{\partial F}{\partial B} \Big|_T$$

E_0 is independent of the magnetic field. We need

$$\frac{\partial}{\partial B} z_M(\eta) = \frac{z'_M(\eta)}{z_M(\eta)} \frac{d\eta}{dB}$$

For the latter derivative we need

$$\begin{aligned} \frac{db}{dB} &= \beta \mu_B \\ \frac{d(2b)}{dB} &= 2\beta \mu_B . \end{aligned}$$

Next we compute

$$\begin{aligned} z'_M(\eta) &= \frac{d}{d\eta} \frac{\sinh(\eta(M + 1/2))}{\sinh(\eta/2)} \\ &= \left(M + \frac{1}{2}\right) \frac{\cosh(\eta(M + 1/2))}{\sinh(\eta/2)} - \frac{1}{2} \frac{\sinh(\eta(M + 1/2)) \cosh(\eta/2)}{\sinh^2(\eta/2)} . \end{aligned}$$

Then

$$\begin{aligned} \frac{z'_M(\eta)}{z_M(\eta)} &= \left(M + \frac{1}{2}\right) \coth(\eta(M + 1/2)) - \frac{1}{2} \coth(\eta/2) \\ &= M \left(\frac{2M + 1}{2M} \coth\left(\frac{M\eta(2M + 1)}{2M}\right) \right) - \frac{1}{2M} \coth\left(\frac{M\eta}{2M}\right) . \end{aligned}$$

Finally we have

$$\frac{z'_M(\eta)}{z_M(\eta)} = M \mathcal{B}_M(M\eta) , \quad (6.16)$$

with

BRILLOUIN FUNCTION	
$\mathcal{B}_M(x) = \frac{2M + 1}{2M} \coth\left(\frac{x(2M + 1)}{2M}\right) - \frac{1}{2M} \coth\left(\frac{x}{2M}\right)$	(6.17)
	(6.18)

Then the final result reads

$$\frac{\mathbf{M}}{N} = \mathbf{e}_z \mu_B B \left(L_0 \mathcal{B}_{L_0}(bL_0) + 2S_0 \mathcal{B}_{S_0}(2bS_0) \right) . \quad (6.19)$$

Properties of the Brillouin function

For small or large arguments, $\coth(x)$ behave like

$$\begin{aligned} x \ll 1 : \quad & \coth(x) = \frac{1}{x} + \frac{x}{3} - \frac{x^3}{45} O(x^5) \\ x \rightarrow \infty : \quad & \coth(x) \rightarrow 1 . \end{aligned}$$

Hence, we have for $x \ll 1$ (MATHEMATICA)

$$\mathcal{B}_M(x) = \frac{M+1}{3M} x - \frac{2M^3 + 4M^2 + 3M + 1}{90M^3} x^3 . \quad (6.20)$$

And for $x \rightarrow \infty$

$$\mathcal{B}_M(x) \rightarrow \frac{2M+1}{2M} - \frac{1}{2M} = 1 .$$

In summary

$$\begin{aligned} \eta \ll 1 : \quad & \mathcal{B}_M(\eta) = \frac{M+1}{3M} \eta \\ \eta \rightarrow \pm\infty : \quad & \mathcal{B}_M(\eta) \rightarrow \pm 1 . \end{aligned}$$

This yields for the magnetization in equation (6.19) [\[previous page\]](#)

$$\begin{aligned} b \ll 1 : \quad \frac{\mathbf{M}}{N} &= \mathbf{e}_z \mu_B \left(L_0 \frac{L_0 + 1}{3L_0} (bL_0) + 2S_0 \frac{S_0 + 1}{3S_0} (2bS_0) \right) \\ &= \mathbf{e}_z \frac{\mu_B^2 B}{3k_B T} \left(L_0(L_0 + 1) + 4S_0(S_0 + 1) \right) \end{aligned}$$

The susceptibility then reads

CURIE LAW
$\chi_{\mu\nu} = \delta_{\mu\nu} \frac{C}{T} , \quad (6.21)$

with

$$C = \frac{\mu_0 \mu_B^2}{3k_B} \left(L_0(L_0 + 1) + 4S_0(S_0 + 1) \right)$$

We still need to consider the large b limit. Here we have

$$b \rightarrow \infty : \quad \frac{\mathbf{M}}{N} \rightarrow \pm \mathbf{e}_z \mu_B (L_0 + 2S_0) .$$

Brillouin function for $M = 1/2$ and $M = \infty$

An important special case is given for spin-1/2, then

$$\begin{aligned}
 \mathcal{B}_{1/2}(x) &= 2 \coth(2x) - \coth(x) \\
 &= \frac{2(e^{2x} + e^{-2x})}{e^{2x} - e^{-2x}} - \frac{e^x + e^{-x}}{e^x - e^{-x}} \cdot \frac{e^x + e^{-x}}{e^x + e^{-x}} \\
 &= \frac{2e^{2x} + 2e^{-2x} - e^{2x} - e^{-2x} - 2}{(e^x - e^{-x})(e^x + e^{-x})} \\
 &= \frac{e^{2x} + e^{-2x} - 2}{(e^x - e^{-x})(e^x + e^{-x})} .
 \end{aligned}$$

So we finally have

$$\mathcal{B}_{1/2}(x) = \tanh(x) \quad (6.22)$$

For large spin ($M \gg 1$) with $\varepsilon = 1/2M \ll 1$ find

$$\begin{aligned}
 \mathcal{B}_M(x) &= (1 + \varepsilon) \coth(x + \varepsilon x) - \varepsilon \coth(\varepsilon x) \\
 &= \coth(x) + \mathcal{O}(\varepsilon) - \frac{\varepsilon}{\varepsilon x} + \mathcal{O}(\varepsilon)
 \end{aligned}$$

Hence

$$\mathcal{B}_{M \rightarrow \infty}(x) = \coth(x) - \frac{1}{x} : \quad (6.23a)$$

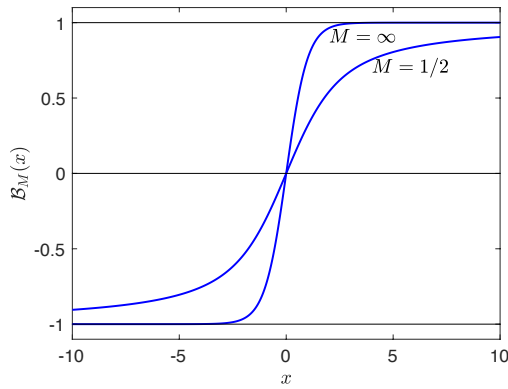


Figure 6.1: .

This is the classical limit.

6.3.2 Strong spin-orbit coupling

To avoid confusion we mark operators by hats. If the spin-orbit coupling is strong compared to the magnetic field, then we cannot ignore the spin-orbit term. In this case, H still commutes with L and S , but no longer with L^z and S^z . Instead, based on the relations

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}} \quad (6.24)$$

$$\hat{\mathbf{L}}\hat{\mathbf{S}} = \frac{1}{2} \left(\hat{\mathbf{J}}^2 - \hat{\mathbf{L}}^2 - \hat{\mathbf{S}}^2 \right), \quad (6.25)$$

H now commutes with L^2, S^2, J^2, J_z . The eigenvectors are therefore

$$|\kappa, L, S, J, J_z\rangle.$$

The corresponding eigenvalues are given by equation (6.11) [p. 144] as

$$E(\kappa, L, S, J, J_z) = E_0(\kappa, L, S) + \frac{B\mu_B}{\hbar} \left(J_z - \langle \hat{S}^z \rangle \right).$$

Here $\langle \hat{S}^z \rangle$ is the expectation value of \hat{S}^z in one of the eigenstates $|\kappa, L, S, J, J_z\rangle$, while J_z is already the eigenvalue of the operator \hat{J}^z . The computation of the expectation value $\langle \hat{S}_z \rangle$ yields eventually

$$\begin{aligned} E(\kappa, L, S, J, J_z) &= E_0(\kappa, L, S) + \underbrace{\frac{\mu_B B}{\hbar} \left(1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \right)}_{=g_J} J_z \\ &= E_0(\kappa, L, S) + \mu_B B g_J m, \end{aligned}$$

with $J_z = \hbar m$ and $m \in \{-J, -J+1, \dots, J\}$

proof

To compute the expectation value we proceed as follows. We start out with the identity

$$\hat{\mathbf{S}} (\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}) - (\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}) \hat{\mathbf{S}} = -i\hbar \hat{\mathbf{S}} \times \hat{\mathbf{L}}. \quad (6.26)$$

which follows from

$$\begin{aligned} \hat{S}_\nu \hat{L}_\mu \hat{S}_\mu - \hat{L}_\mu \hat{S}_\mu \hat{S}_\nu &= \hat{S}_\nu \hat{S}_\mu \hat{L}_\mu - \hat{S}_\mu \hat{S}_\nu \hat{L}_\mu = [\hat{S}_\nu, \hat{S}_\mu] \hat{L}_\mu \\ &= i\hbar \varepsilon_{\nu\mu\rho} \hat{S}_\rho \hat{L}_\mu = -i\hbar \varepsilon_{\nu\rho\mu} \hat{S}_\rho \hat{L}_\mu \\ &= -i\hbar (\hat{\mathbf{S}} \times \hat{\mathbf{L}})_\nu \end{aligned}$$

. Next we multiply equation (6.26) with $\times \hat{\mathbf{J}}$ and obtain

$$\hat{\mathbf{S}} (\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}) \times \hat{\mathbf{J}} - (\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}) \hat{\mathbf{S}} \times \hat{\mathbf{J}} = -i\hbar (\hat{\mathbf{S}} \times \hat{\mathbf{L}}) \times \hat{\mathbf{J}} \quad (6.27)$$

Now, $(\hat{\mathbf{L}} \cdot \hat{\mathbf{S}})$ commutes with all components of the vector operator $\hat{\mathbf{J}}$, since according to equation (6.27) [next page](#) $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$ is given by $\frac{1}{2}(\hat{\mathbf{J}}^2 - \hat{\mathbf{L}}^2 - \hat{\mathbf{S}}^2)$ which can be seen as follows

$$\begin{aligned} [\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}, J^\alpha] &= \frac{1}{2} \left(\underbrace{[J^2, J^\alpha]}_{=0} - [L^2, J^\alpha] - [S^2, J^\alpha] \right) \\ &= -\frac{1}{2} \left([L^2, L^\alpha + S^\alpha] + [S^2, L^\alpha + S^\alpha] \right) \\ &= -\frac{1}{2} \left([L^2, L^\alpha] + [S^2, S^\alpha] \right) \\ &= 0 . \end{aligned}$$

Then we can move $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$ in the first term of equation (6.27) to the right of $\hat{\mathbf{J}}$, resulting in

$$(\hat{\mathbf{S}} \times \hat{\mathbf{J}}) (\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}) - (\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}) (\hat{\mathbf{S}} \times \hat{\mathbf{J}}) = -i\hbar (\hat{\mathbf{S}} \times \hat{\mathbf{L}}) \times \hat{\mathbf{J}}$$

If we now compute expectation values in the eigenvectors $|\kappa, L, S, J, J_z\rangle$, we can replace the operators $(\hat{\mathbf{L}} \cdot \hat{\mathbf{S}})$ by the eigenvalues $\frac{1}{2}(J(J+1) - L(L+1) - S(S+1))$ and the remaining expectation value on the left hand side is zero. Hence, we obtain from the right hand side

$$\langle (\hat{\mathbf{S}} \times \hat{\mathbf{L}}) \times \hat{\mathbf{J}} \rangle = 0 , \quad (6.28)$$

which is valid in the eigenstates. From

$$\begin{aligned} [(\hat{\mathbf{S}} \times \hat{\mathbf{L}}) \times \hat{\mathbf{J}}]_i &= \varepsilon_{ijk} (\hat{\mathbf{S}} \times \hat{\mathbf{L}})_j \hat{J}_k \\ &= \varepsilon_{ijk} \varepsilon_{jmn} \hat{S}_m \hat{L}_n \hat{J}_k \\ &= \varepsilon_{jki} \varepsilon_{jmn} \hat{S}_m \hat{L}_n \hat{J}_k \\ &= (\delta_{km} \delta_{in} - \delta_{kn} \delta_{im}) \hat{S}_m \hat{L}_n \hat{J}_k \\ &= \hat{S}_k \hat{L}_i \hat{J}_k - \hat{S}_i \hat{L}_k \hat{J}_k \\ &= \hat{L}_i \hat{S}_k \hat{J}_k - \hat{S}_i \hat{L}_k \hat{J}_k . \end{aligned}$$

we obtain for the double vector product

$$\begin{aligned} (\hat{\mathbf{S}} \times \hat{\mathbf{L}}) \times \hat{\mathbf{J}} &= \hat{\mathbf{L}} (\hat{\mathbf{S}} \cdot \hat{\mathbf{J}}) - \hat{\mathbf{S}} (\hat{\mathbf{L}} \cdot \hat{\mathbf{J}}) \\ &= (\hat{\mathbf{J}} - \hat{\mathbf{S}}) (\hat{\mathbf{S}} \cdot \hat{\mathbf{J}}) - \hat{\mathbf{S}} (\hat{\mathbf{L}} \cdot \hat{\mathbf{J}}) \\ &= \hat{\mathbf{J}} (\hat{\mathbf{S}} \cdot \hat{\mathbf{J}}) - \hat{\mathbf{S}} ((\hat{\mathbf{L}} + \hat{\mathbf{S}}) \cdot \hat{\mathbf{J}}) \\ &= \hat{\mathbf{J}} (\hat{\mathbf{S}} \cdot \hat{\mathbf{J}}) - \hat{\mathbf{S}} \hat{\mathbf{J}}^2 . \end{aligned}$$

From equation (6.28) we therefore obtain

$$(\hat{\mathbf{S}} \times \hat{\mathbf{L}}) \times \hat{\mathbf{J}} = \hat{\mathbf{J}} (\hat{\mathbf{S}} \cdot \hat{\mathbf{J}}) - \hat{\mathbf{S}} \hat{\mathbf{J}}^2 = 0 .$$

and for the expectation value in the eigenstates $|\kappa, L, S, J, J^z\rangle$ we have

$$\langle \hat{J}_z (\hat{\mathbf{S}} \cdot \hat{\mathbf{J}}) \rangle - \langle \hat{S}_z J^2 \rangle = 0 .$$

Next we use

$$\begin{aligned} \hat{\mathbf{S}} \cdot \hat{\mathbf{J}} &= \hat{\mathbf{S}} \cdot \hat{\mathbf{L}} + \hat{\mathbf{S}}^2 \\ &= \frac{1}{2}(\hat{\mathbf{J}}^2 - \hat{\mathbf{S}}^2 - \hat{\mathbf{L}}^2) + \hat{\mathbf{S}}^2 \\ &= \frac{1}{2}(\hat{\mathbf{J}}^2 + \hat{\mathbf{S}}^2 - \hat{\mathbf{L}}^2) . \end{aligned}$$

and obtain

$$\begin{aligned} J_z \frac{1}{2} \langle \hat{\mathbf{J}}^2 + \hat{\mathbf{S}}^2 - \hat{\mathbf{L}}^2 \rangle - \langle \hat{S}_z J(J+1) \rangle &= 0 \\ J_z \frac{1}{2} (J(J+1) + S(S+1) - L(L+1)) - \langle \hat{S}_z \rangle J(J+1) &= 0 . \end{aligned}$$

The expectation value $\langle S_z \rangle$ in the eigenstates $|\kappa, L, S, J, J^z\rangle$ is therefore:

$$\langle S_z \rangle = J_z \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} .$$

Hence, the eigenvalues are

$$E(\kappa, L, S, J, J_z) = E_0(\kappa, L, S) + \frac{\mu_B B}{\hbar} \underbrace{\left(1 + \frac{1}{2} [J(J+1) + S(S+1) - L(L+1)] \right)}_{=g_J} J_z .$$

q.e.d. ✓

The remaining calculation is similar to the previous one and one obtains

$$\frac{F}{N} = E_0 - k_B T \ln \left(z_J(b) \right)$$

with $b = g_J \mu_B \beta B$. Then

$$\hat{\mathbf{M}} = \mathbf{e}_z N J g_J \mu_B B \mathcal{B}_J(bJ) .$$

For high T and small B , the susceptibility yields

CURIE LAW
$\chi_{\mu\nu} = \delta_{\mu\nu} \frac{C}{T} . \quad (6.29)$

with

$$C = \frac{N\mu_0\mu_B^2 g_J^2 J(J+1)}{3k_B} ,$$

and for large b we have

$$\frac{\mathbf{M}}{N} \xrightarrow{b \rightarrow \infty} \pm \mathbf{e}_z g_J \mu_B J .$$

Plot of the Brillouin function

Entropy

For the entropy we obtain

$$\frac{S}{N} = - \frac{\partial F/N}{\partial T} \Big|_{\mathbf{B}} = k_B \ln(z_J(b)) + k_B T \frac{z'_J(b)}{z_J(b)} \frac{db}{dT}$$

$$\frac{db}{dT} = -g_J \mu_B B \frac{1}{k_B T^2} = -\beta^2 g_J \mu_B B = -\beta b .$$

$$S = k_B \left(\ln(z_J(b)) - b \frac{z'_J(b)}{z_J(b)} \right)$$

Along with equation (6.16) [\[p. 146\]](#) we obtain

$$\frac{S}{N} = k_B \left(\ln \left(\frac{\sinh(b(J+1/2))}{\sinh(b/2)} \right) - b J \mathcal{B}_J(bJ) \right) .$$

For $b \ll 1$ (i.e. $T \rightarrow \infty$) we find

$$\begin{aligned} \frac{S}{N} &= k_B \left(\ln \left(\frac{b(J+1/2)}{b/2} \right) - (bJ)^2 \frac{J+1}{3J} \right) \\ &= k_B \ln(2J+1) . \end{aligned}$$

The argument is the number of eigenvalues of J_z .

6.3.3 Plot of S and specific heat

6.4 Magnetism of the free electron model

The free electron gas is based on the following assumptions: no electron-electron interactions, the electrons experience no potential due to the crystal, they are confined to a box. In addition, we apply a constant homogeneous external magnetic field.

6.4.1 Pauli paramagnetism

First, we restrict the discussion to the coupling of the electronic spin to the magnetic field, i.e. we ignore the angular momentum. The energy one-particle eigenvalues are

$$\begin{aligned}\varepsilon_\sigma(\mathbf{k}) &= \frac{\hbar^2 \mathbf{k}^2}{2m} + \sigma b, \\ b &= \frac{\mu_B g_e}{2} B.\end{aligned}$$

with the quantized wave vectors \mathbf{k} . The mean occupation of the one-particle orbitals is given by the Fermi-Dirac distribution

$$n_F(\varepsilon_\sigma(\mathbf{k})|T, \mu)$$

The mean total number of electrons in the Zeeman level represented by σ is

$$N_\sigma = \sum_{\mathbf{k}} n_F(\varepsilon_\sigma(\mathbf{k})|T, \mu) = \int d\varepsilon \rho(\varepsilon) n_F(\varepsilon + \sigma b|T, \mu).$$

As derived in appendix (8.3) the 3D dos is

$$\rho(\varepsilon) = D\sqrt{\varepsilon}, \quad (6.30a)$$

$$\text{with } D = \frac{Vm^{3/2}}{\hbar^3 \pi^2 \sqrt{2}}. \quad (6.30b)$$

Then

$$N_\sigma = D \int_0^\infty d\varepsilon \sqrt{\varepsilon} n_F(\varepsilon + \sigma b|T, \mu).$$

For small magnetic field we can use a Taylor expansion in b around $b = 0$

$$\begin{aligned}N_\sigma &= D \int_0^\infty d\varepsilon \sqrt{\varepsilon} \left(n_F(\varepsilon|T, \mu) + \sigma b \frac{\partial}{\partial \varepsilon} n_F(\varepsilon|T, \mu) + \mathcal{O}(b^2) \right) \\ &= D \int_0^\infty d\varepsilon \sqrt{\varepsilon} n_F(\varepsilon|T, \mu) + \sigma b D \int_0^\infty d\varepsilon \sqrt{\varepsilon} n'_F(\varepsilon|T, \mu) + \mathcal{O}(b^2)\end{aligned}$$

The total particle number follows as

$$\begin{aligned} N &= N_+ + N_- = 2D \int_0^\infty d\varepsilon \sqrt{\varepsilon} n_F(\varepsilon|T, \mu) + \mathcal{O}(b^2) \\ &= 2D \int_0^\infty d\varepsilon \sqrt{\varepsilon} n_F(\varepsilon|T, \mu) + \mathcal{O}(b^2) . \end{aligned} \quad (6.31)$$

For small b and low temperature we can use the Sommerfeld expansion, outlined in appendix (8.1),

SOMMERFELD EXPANSION	
$\begin{aligned} I &= \int_0^\infty f(\varepsilon) n_F(\varepsilon \mu, T) d\varepsilon \\ &= \int_0^\mu f(\varepsilon) d\varepsilon + 2 \sum_{n=1}^{\text{odd}} \left(1 - \frac{1}{2^n}\right) \zeta(n+1) (k_B T)^{n+1} f^{(n)}(\mu) , \end{aligned} \quad (6.32)$	(6.32)

which reads to leading order

$$I = \int_0^\mu f(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 f'(\mu) + \mathcal{O}\left(\left(\frac{k_B T}{\mu}\right)^4\right) .$$

For the total particle number we obtain

$$\begin{aligned} N &= 2D \left(\int_0^\mu \sqrt{\varepsilon} + \frac{\pi^2}{6} \frac{d}{d\mu} \sqrt{\mu} (k_B T)^2 + \dots \right) \\ &= 2D \left(\frac{2}{3} \mu^{3/2} + \frac{\pi^2}{12} \mu^{-1/2} (k_B T)^2 + \dots \right) . \\ \frac{3N}{4D} &= \mu^{3/2} \left(1 + \frac{\pi^2}{8} \left(\frac{k_B T}{\mu} \right)^2 + \dots \right) \end{aligned} \quad (6.33)$$

For $T = 0$ the chemical potential is equivalent to the Fermi energy ε_F and we have

$$\frac{3N}{4D} = \varepsilon_F^{3/2} , \quad (6.34)$$

or rather

$$\varepsilon_F = \left(\frac{3N \hbar^3 (2\pi)^2}{4V (2m)^{3/2}} \right)^{2/3} = \left(\frac{3N \pi^2}{V} \right)^{2/3} \frac{\hbar^2}{2m} .$$

FERMI ENERGY IN THE FREE ELECTRON GAS

$$\varepsilon_F = \left(3\pi^2 n\right)^{2/3} \frac{\hbar^2}{2m} . \quad (6.35)$$

This defines the Fermi wave number k_F , through

$$\begin{aligned} \varepsilon_F &= \left(3\pi^2 n\right)^{2/3} \frac{\hbar^2}{2m} = \frac{\hbar^2 k_F^2}{2m} \\ k_F &= \left(3\pi^2 n\right)^{1/3} = \left(\frac{3\pi^2}{v}\right)^{1/3} , \end{aligned}$$

where v is the average volume per electron. Hence

$$k_F \propto \frac{1}{r} ,$$

where r is the mean distance between the electrons. Inserting equation (6.34) [\[previous page\]](#) in equation (6.33) [\[previous page\]](#) yields apart from higher order terms

$$\begin{aligned} \varepsilon_F &= \mu \left(1 + \frac{\pi^2}{8} \left(\frac{k_B T}{\mu}\right)^2\right)^{2/3} \\ \mu &= \varepsilon_F \left(1 + \frac{\pi^2}{8} \left(\frac{k_B T}{\mu}\right)^2\right)^{-2/3} . \end{aligned}$$

We can solve this equation iteratively, starting with $\mu = \varepsilon_F$. The first iteration yields

$$\mu = \varepsilon_F \left(1 + \frac{\pi^2}{8} \left(\frac{k_B T}{\varepsilon_F}\right)^2\right)^{-2/3} .$$

For low temperatures, $\frac{k_B T}{\varepsilon_F} < 1$ we can as well write

$$\mu = \varepsilon_F \left(1 - \frac{\pi^2}{8} \frac{2}{3} \left(\frac{k_B T}{\varepsilon_F}\right)^2 + \mathcal{O}\left(\left(\frac{k_B T}{\varepsilon_F}\right)^4\right)\right) .$$

Further iterations do not change the second order term and we generally have

CHEMICAL POTENTIAL (free electron gas)	
$\mu = \varepsilon_F \left(1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F} \right)^2 \right) + \mathcal{O} \left(\left(\frac{k_B T}{\varepsilon_F} \right)^4 \right)$	(6.36)

The partition function for non-interacting particles has already been derived previously. For one-particle energies ε_ν it was

$$\ln(Z) = \sum_{\nu} \ln \left(1 + e^{-\beta(\varepsilon_\nu - \mu)} \right).$$

In the present case the index ν stands for the wave vector \mathbf{k} and the spin direction. Hence

$$\ln(Z) = \sum_{\sigma} \int_0^{\infty} \rho(\varepsilon) \ln \left(1 + e^{-\beta(\varepsilon + \sigma b - \mu)} \right). \quad (6.37)$$

The corresponding grand potential reads

$$\Omega(T, \mathbf{B}) = -k_B T \ln(Z) = -k_B T \sum_{\sigma} \int_0^{\infty} \rho(\varepsilon) \ln \left(1 + e^{-\beta(\varepsilon + \sigma b - \mu)} \right).$$

The magnetization in z-direction is obtain via

$$\begin{aligned}
 M &= - \left. \frac{\partial \Omega}{\partial B} \right|_T \\
 &= k_B T \sum_{\sigma} \left(- \frac{\beta \sigma \mu_B g_e}{2} \right) \int_0^{\infty} d\varepsilon \rho(\varepsilon) \frac{e^{-\beta(\varepsilon + \sigma b - \mu)}}{1 + e^{-\beta(\varepsilon + \sigma b - \mu)}} \\
 &= - \frac{\mu_B g_e}{2} \sum_{\sigma} \sigma \int_0^{\infty} d\varepsilon \rho(\varepsilon) n_F(\varepsilon + \sigma b | T, \mu) \\
 &= - \frac{\mu_B g_e}{\hbar} \underbrace{\frac{\hbar(N_+ - N_-)}{2}}_{=\langle S_{\text{total}}^z \rangle}
 \end{aligned}$$

In agreement with equation (6.2) [p. 137]. Again we assume that b is small

and employ a Taylor expansion.

$$\begin{aligned}
M &= -\frac{\mu_B g_e}{2} \sum_{\sigma} \sigma \int_0^{\infty} d\varepsilon \left(\rho(\varepsilon) n_F(\varepsilon|T, \mu) + \sigma b n'_F(\varepsilon|T, \mu) + O(b^2) \right) \\
&= -\frac{\mu_B g_e}{2} 2b \int_0^{\infty} d\varepsilon \rho(\varepsilon) n'_F(\varepsilon|T, \mu) + O(b^2) \\
&= -\frac{(\mu_B g_e)^2}{2} B \int_0^{\infty} d\varepsilon \rho(\varepsilon) n'_F(\varepsilon|T, \mu) + O(b^2) .
\end{aligned}$$

Then the susceptibility reads

$$\begin{aligned}
\chi_T &= \mu_0 \left. \frac{\partial M}{\partial B} \right|_T \Big|_{B=0} \\
&= -\mu_0 \frac{(\mu_B g_e)^2}{2} \int_0^{\infty} d\varepsilon \rho(\varepsilon) n'_F(\varepsilon|T, \mu) .
\end{aligned}$$

This can also be written as

$$\begin{aligned}
\chi_T &= -\mu_0 \mu_B^2 \left(\frac{g_e}{2} \right)^2 2 \int d\varepsilon \rho(\varepsilon) n'_F(\varepsilon|T, \mu) \\
&= \mu_0 \mu_B^2 \left(\frac{g_e}{2} \right)^2 2 \frac{\partial}{\partial \mu} \int d\varepsilon \rho(\varepsilon) n_F(\varepsilon|T, \mu) .
\end{aligned}$$

Comparison with equation (6.31) [p. 154] yields

$$\chi_T = \mu_0 \mu_B^2 \left(\frac{g_e}{2} \right)^2 \left. \frac{\partial N}{\partial \mu} \right|_{T, B=0} \quad (6.38)$$

We use the Sommerfeld expansion, derived in appendix (8.1) to expand the integral in powers of $k_B T / \mu$.

$$\begin{aligned}
\chi &= -\mu_0 \frac{(\mu_B g_e)^2}{2} \int_0^{\infty} d\varepsilon \rho(\varepsilon) n'_F(\varepsilon|T, \mu) \\
&= \mu_0 \frac{(\mu_B g_e)^2}{2} \int_0^{\infty} d\varepsilon \rho'(\varepsilon) n_F(\varepsilon|T, \mu) \\
&= \mu_0 \frac{(\mu_B g_e)^2}{2} \left(\int_0^{\mu} d\varepsilon \rho'(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 \rho''(\mu) + \mathcal{O}\left(\left(\frac{k_B T}{\mu}\right)^4\right) \right) \\
&= \mu_0 \frac{(\mu_B g_e)^2}{2} \left(\rho(\mu) + \frac{\pi^2}{6} (k_B T)^2 \rho''(\mu) + \mathcal{O}\left(\left(\frac{k_B T}{\mu}\right)^4\right) \right) .
\end{aligned}$$

The final result reads

$$\chi = \mu_0 \frac{(\mu_B g_e)^2}{2} \rho(\mu) \left(1 + \frac{\pi^2}{6} (k_B T)^2 \frac{\rho''(\mu)}{\rho(\mu)} + \dots \right) \quad (6.39)$$

Now we recall, that $\rho(\varepsilon) = D\sqrt{\varepsilon}$, resulting in $\rho''(\mu)/\rho(\mu) = -1/(4\mu^2)$.

MAGNETIC SUSCEPTIBILITY (free electron gas)	
$\chi_P = \mu_0 \frac{(\mu_B g_e)^2}{2} \rho(\mu) \left(1 - \frac{\pi^2}{24} \left(\frac{k_B T}{\mu} \right)^2 + \dots \right).$	(6.40)

We see that indeed $k_B T/\mu$ is the relevant small parameter. This describes the **Pauli-spin-paramagnetism**, which is almost temperature independent for low T ; in strong contrast to the Curie $1/T$ behaviour. The reason for the discrepancy lies in the fermi-statistics. Only the spin of the electrons in the vicinity of μ can contribute. The number of thermally excited electrons is $k_B T \rho(\mu)$ which compensates the $1/T$ behaviour.

6.4.2 Langevin Diamagnetismus

So far we have only considered the spin degrees of freedom of the free electron gas. The orbital moments also contribute to the magnetization, which results in the

LANDAU DIAMAGNETISM (free electron gas)	
$\chi_L = -\frac{1}{3}\chi_P$	(6.41)

For the derivation see appendix ??

6.5 Collective magnetism

6.5.1 Heisenberg hamiltonian

In many crystalline systems, the electrons can be split into those that are localized at the atomic sites and others which can move freely through the

crystal. The former result in localized magnetic moments or spins \mathbf{S}_i , if they do not belong to closed shells. We have discussed these local spins \mathbf{S}_i before, but there we have focussed on systems where these spins do not interact. The Coulomb interaction between the electrons can lead to various types of exchange interactions between these spins. The exchange can either result from exchange processes of the electrons that form the local spins on neighboring sites *direct exchange* or it can be mediated by additional electrons *indirect exchange*. In the latter case, the interaction can be long ranged, like in the case of the so-called *RKKY* (Ruderman-Kittel-Kasuya-Yosida). In RKKY the interaction decays like $1/|\mathbf{R}_i - \mathbf{R}_j|^3$ with the distance between the spins at site \mathbf{R}_i and \mathbf{R}_j . In addition, the exchange interaction changes sign as function of distance, i.e. depending on the distance between the localized spins it can be ferromagnetic and anti-ferromagnetic. In all cases, the interaction can be described by a prominent model for collective magnetism, the

HEISENBERG MODEL	
$H = - \sum_{jj'} \left(J_{jj'}^z S_j^z S_{j'}^z + J_{jj'}^{xy} (S_j^x S_{j'}^x + S_j^y S_{j'}^y) \right) + b \sum_j S_j^z . \quad (6.42)$	

Here $J_{jj'} = J(|\mathbf{R}_j - \mathbf{R}_{j'}|)$, with $J_{jj} = 0$. $J_{jj'}$ can always be chosen symmetric, since by substituting $j \leftrightarrow j'$ we find

$$H_H = - \sum_{\alpha} \sum_{jj'} J_{jj'} S_j^{\alpha} S_{j'}^{\alpha} = - \sum_{\alpha} \sum_{jj'} J_{j'j} S_{j'}^{\alpha} S_j^{\alpha} = - \sum_{\alpha} \sum_{jj'} J_{j'j} S_j^{\alpha} S_{j'}^{\alpha}$$

Hence

$$H = \frac{1}{2} \left(- \sum_{\alpha} \sum_{jj'} J_{jj'} S_j^{\alpha} S_{j'}^{\alpha} + - \sum_{\alpha} \sum_{jj'} J_{j'j} S_{j'}^{\alpha} S_j^{\alpha} \right) = - \sum_{\alpha} \sum_{jj'} \left(\frac{J_{jj'} + J_{j'j}}{2} \right) S_j^{\alpha} S_{j'}^{\alpha} .$$

We also introduce the ladder operators

$$S_j^{\pm} = S_j^x \pm i S_j^y . \quad (6.43)$$

In these operators, the hamiltonian reads

$$H = - \sum_{jj'} \left(J_{jj'}^z S_j^z S_{j'}^z + J_{jj'}^{xy} S_j^+ S_{j'}^- \right) + b \sum_j S_j^z .$$

The order of the operators $S_j^+ S_{j'}^-$ is irrelevant, since $j \neq j'$ and in that case they commute. There are three important limiting cases depending on the anisotropy of the crystal in spin-space.

- ($|J^z| \ll |J^{xy}|$) results in the so-called *xy-model*

XY-MODEL
$H = - \sum_{jj'} J_{jj'}^{xy} S_j^+ S_{j'}^- + b \sum_j S_j^z . \quad (6.44)$

- ($|J^z| \gg |J^{xy}|$) results in the so-called *Ising model*, which is discussed in great detail chapter chapter (1) [\[page 4\]](#)
- ($J^z = J^{xy}$) represents the isotropic Heisenberg model

HEISENBERG MODEL (<i>isotropic case</i>)
$H = - \sum_{jj'} J_{jj'} \mathbf{S}_j \cdot \mathbf{S}_{j'} + b \sum_j S_j^z . \quad (6.45)$

Very often the exchange coupling $J_{jj'} = J(|\mathbf{R}_j - \mathbf{R}_{j'}|)$ decreases very rapidly with distance and it suffices to take only nearest neighbour (nn) interactions into account, i.e.

$$- \sum_{jj'} J_{jj'} \approx -J \sum_{\langle jj' \rangle} . \quad (6.46)$$

In general, J can be positive or negative. In the first (second) case, ferromagnetic (anti-ferromagnetic) spin alignment is favoured. If the exchange coupling between localized spins is mediated by itinerant electrons, the so-called *RKKY-interaction* (Ruderman-Kittel-Kasuya-Yosida) results, which is long

ranged and oscillating as function of distance, i.e. depending on the distance between the localized spins it can be ferromagnetic and anti-ferromagnetic.

6.5.2 Mermin-Wagner Theorem

There are only a few exact results available for the Heisenberg model. Presumably the most important one is due to Mermin and Wagner and states: *In one and two dimensions, continuous symmetries cannot be broken spontaneously at finite temperature in systems with sufficiently short-ranged interactions.*

The proof of the Mermin-Wagner theorem is based on the

BOGOLIUBOV INEQUALITY	
$\frac{\beta}{2} \langle [A, A^\dagger]_+ \rangle .$	(6.47)

Here, H stands for the hamiltonian and A and C for arbitrary operators. $[\bullet, \bullet]_+$ denotes the anti-commutator and $[\bullet, \bullet]_- = [\bullet, \bullet]$ the commutator. The prove is given in appendix (8.6). Now we will apply the Bogoliubov inequality to the isotropic Heisenberg model including an external field

$$\mathbf{B}_j = b \mathbf{e}_z e^{i\mathbf{Q}\mathbf{R}_j} ,$$

that couples to different types of magnetic order (e.g. ferro, anti-ferro), depending on the choice of the wave vector \mathbf{Q} .

We consider the order parameter is defined as

$$\mathcal{S}_{\mathbf{Q}}(T, b) = \frac{1}{\hbar N} \langle \mathbf{S}_{\mathbf{Q}}^z \rangle_{T, b} . \quad (6.48)$$

The operator $S_{\mathbf{Q}}^z$ stands for the Fourier transform of S_j^z , defined in equation (6.52) [next page](#) .

The results after a straightforward but tedious calculation reads

$$1D) \quad |\mathcal{S}_{\mathbf{Q}}(T, b)| \leq \left(\frac{|b|}{T^2} \right)^{1/3} \xrightarrow{b \rightarrow 0} 0 \quad (6.49a)$$

$$2D) \quad |\mathcal{S}_{\mathbf{Q}}(T, b)| \leq \frac{const}{\sqrt{T}} \frac{const}{\sqrt{T |\ln(|b|)|}} \xrightarrow{b \rightarrow 0} 0 \quad (6.49b)$$

$$3D) \quad |\mathcal{S}_{\mathbf{Q}}(T, b)| \quad (6.49c)$$

For finite T the rhs in 1D 2D goes to zero for vanishing field ($b \rightarrow 0$). Hence there is no finite order parameter possible, irrespective of the wve vector \mathbf{Q} (order). For 3D, however, the Mermin-Wagner theorem does not rule out spontaneous magnetization for finite T .

6.5.3 Proof of the Mermin-Wagner Theorem

The hamiltonian reads

$$H = - \sum_{jj'} J_{jj'} \mathbf{S}_j \mathbf{S}_{j'} + b S_{\mathbf{Q}}^z . \quad (6.50)$$

The division by \hbar makes the order parameter dimensionless and the factor $1/N$ leads to the magnetization per site in the ferromagnetic case. The spin operators obey the common commutator relations of angular momenta

$$[S_j^z S_{j'}^\pm] = \pm \delta_{jj'} \hbar S_j^\pm \quad (6.51a)$$

$$[S_j^+ S_{j'}^-] = \delta_{jj'} 2\hbar S_j^z . \quad (6.51b)$$

It is expedient to introduce Fourier transformed operators

$$S_k^\alpha = \sum_j S_j^\alpha e^{i\mathbf{k}\mathbf{R}_j} , \quad \alpha \in \{x, y, z\} \quad (6.52a)$$

$$S_j^\alpha = \frac{1}{N} \sum_k S_k^\alpha e^{-i\mathbf{k}\mathbf{R}_j} \quad (6.52b)$$

From that we obtain

$$S_{\mathbf{k}}^\pm := \sum_j e^{i\mathbf{k}\mathbf{R}_j} S_j^\pm = \sum_j e^{i\mathbf{k}\mathbf{R}_j} (S_j^x \pm i S_j^y) = S_{\mathbf{k}}^x \pm i S_{\mathbf{k}}^y \quad (6.53)$$

The commutation relations in these operators are

$$[S_k^z S_{k'}^\pm] = \pm \hbar S_{k+k'}^\pm \quad (6.54a)$$

$$[S_k^+ S_{k'}^-] = 2\hbar S_{k+k'}^z . \quad (6.54b)$$

We assume that the exchange coupling decays rapidly enough to ensure

$$X := \frac{S(S+1)\hbar^2}{N} \sum_{jj'} |J_{jj'}| |\mathbf{R}_j - \mathbf{R}_{j'}|^2 < \infty , \quad \forall N . \quad (6.55)$$

For the proof of the Mermin-Wagner theorem the following operators are used

$$A = A_{\mathbf{k}} = S_{\mathbf{Q}-\mathbf{k}}^{-}, \quad A_{\mathbf{k}}^{\dagger} = S_{\mathbf{k}-\mathbf{Q}}^{+} \quad (6.56a)$$

$$C = C_{\mathbf{k}} = S_{\mathbf{k}}^{+}, \quad C_{\mathbf{k}}^{\dagger} = S_{-\mathbf{k}}^{-}. \quad (6.56b)$$

The first term in the Bogoliubov inequality that we compute is

$$\langle [C_{\mathbf{k}}, A_{\mathbf{k}}]_{-} \rangle = \langle [S_{\mathbf{k}}^{+}, S_{\mathbf{Q}-\mathbf{k}}^{-}] \rangle = 2\hbar N S_{\mathbf{Q}}^z(T, b). \quad (6.57)$$

The second term that we consider is

$$\sum_{\mathbf{k}} \langle [A_{\mathbf{k}}, A_{\mathbf{k}}^{\dagger}]_{+} \rangle = \sum_{\mathbf{k}} \langle S_{\mathbf{Q}-\mathbf{k}}^{-} S_{\mathbf{k}-\mathbf{Q}}^{+} + S_{\mathbf{k}-\mathbf{Q}}^{+} S_{\mathbf{Q}-\mathbf{k}}^{-} \rangle \quad (6.58)$$

$$= \sum_{jj'} \sum_{\mathbf{k}} e^{i(\mathbf{Q}-\mathbf{k})\mathbf{R}_j} e^{i(\mathbf{k}-\mathbf{Q})\mathbf{R}_{j'}} \langle S_j^{-} S_{j'}^{+} + S_{j'}^{+} S_j^{-} \rangle \quad (6.59)$$

$$= \sum_{jj'} e^{i\mathbf{Q}(\mathbf{R}_j - \mathbf{R}_{j'})} \underbrace{\sum_{\mathbf{k}} e^{-i\mathbf{k}(\mathbf{R}_j - \mathbf{R}_{j'})} \langle S_j^{-} S_{j'}^{+} + S_{j'}^{+} S_j^{-} \rangle}_{=N\delta_{jj'}} \quad (6.60)$$

$$= N \sum_j \langle S_j^{-} S_j^{+} + S_j^{+} S_j^{-} \rangle \quad (6.61)$$

$$= 2N \sum_j \langle (S_y^x)^2 + (S_j^y)^2 \rangle, \quad (6.62)$$

This term can be estimated by

$$\sum_{\mathbf{k}} \langle [A_{\mathbf{k}}, A_{\mathbf{k}}^{\dagger}]_{+} \rangle \leq 2N \sum_j \underbrace{\langle (\mathbf{S}_j)^2 \rangle}_{= \hbar^2 S(S+1)} = 2N^2 \hbar^2 S(S+1),$$

resulting in

$$\beta N^2 \hbar^2 S(S+1) \geq \frac{\beta}{2} \sum_{\mathbf{k}} \langle [A, A^{\dagger}]_{+} \rangle, \quad (6.63)$$

For the remaining term in the Bogoliubov inequality we find (proof in appendix appendix (8.7))

$$4\hbar^2 N (|b S_{\mathbf{Q}}(T, b)| + \mathbf{k}^2 X) \geq \left\langle \left[[C_{\mathbf{k}}, H]_{-}, C_{\mathbf{k}}^{\dagger} \right]_{-} \right\rangle \quad (6.64)$$

with the definition of X in equation (6.55) [\[previous page\]](#). The Bogoliubov inequality reads

$$\frac{\beta}{2} \langle [A_{\mathbf{k}}, A_{\mathbf{k}}^{\dagger}]_{+} \rangle \langle [[C_{\mathbf{k}}, H]_{-}, C_{\mathbf{k}}^{\dagger}]_{-} \rangle \geq |\langle [C_{\mathbf{k}}, A_{\mathbf{k}}]_{-} \rangle|^2$$

According to equation (8.12) [p. 194] the second factor is greater zero, therefore

$$\begin{aligned} \frac{\beta}{2} \langle [A_{\mathbf{k}}, A_{\mathbf{k}}^\dagger]_+ \rangle &\geq \frac{|\langle [C_{\mathbf{k}}, A_{\mathbf{k}}]_- \rangle|^2}{\langle [[C_{\mathbf{k}}, H]_-, C_{\mathbf{k}}^\dagger]_- \rangle} \\ \Rightarrow \quad \frac{\beta}{2} \sum_{\mathbf{k}} \langle [A_{\mathbf{k}}, A_{\mathbf{k}}^\dagger]_+ \rangle &\geq \sum_{\mathbf{k}} \frac{|\langle [C_{\mathbf{k}}, A_{\mathbf{k}}]_- \rangle|^2}{\langle [[C_{\mathbf{k}}, H]_-, C_{\mathbf{k}}^\dagger]_- \rangle}. \end{aligned}$$

Finally, we use the operators in equation (6.56) [previous page] in the Bogoliubov inequality, sum over \mathbf{k} and use equation (6.57) [previous page], equation (6.63) [previous page] and equation (6.64) [previous page], resulting in

$$\begin{aligned} \beta N^2 \hbar^2 S(S+1) &\geq \frac{\beta}{2} \sum_{\mathbf{k}} \langle [A_{\mathbf{k}}, A_{\mathbf{k}}^\dagger]_+ \rangle \\ &\geq \sum_{\mathbf{k}} \frac{|[C_{\mathbf{k}}, A_{\mathbf{k}}]_-|^2}{\langle [[C_{\mathbf{k}}, H]_-, C_{\mathbf{k}}^\dagger]_- \rangle} \\ \beta N^2 \hbar^2 S(S+1) &\geq \frac{4\hbar^2 N^2 \mathcal{S}_{\mathbf{Q}}^2(T, b)}{4N} \sum_{\mathbf{k}} \frac{1}{|b\mathcal{S}_{\mathbf{Q}}(T, b)| + \mathbf{k}^2 X} \\ \beta S(S+1) &\geq \frac{\mathcal{S}_{\mathbf{Q}}(T, b)}{N} \sum_{\mathbf{k}} \frac{1}{|b\mathcal{S}_{\mathbf{Q}}(T, b)| + \mathbf{k}^2 X} \\ \beta S(S+1) &\geq \mathcal{S}_{\mathbf{Q}}^2(T, b) I, \end{aligned}$$

with

$$\begin{aligned} I &:= \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{|b\mathcal{S}_{\mathbf{Q}}(T, b)| + \mathbf{k}^2 X} \\ &= \frac{V}{N(2\pi)^D} \int_{V_{1bc}} d^D k \frac{1}{|b\mathcal{S}_{\mathbf{Q}}(T, b)| + \mathbf{k}^2 X} \end{aligned}$$

The volume V_{1bc} of integration is the first Brillouin zone of a simple square lattice, i.e. a D -dimensional cube with edges ranging from $-\pi$ to π . Since the integrand is positive, the integral becomes smaller, if we replace the volume

by that of a sphere, V_{sp} , that lies entirely within V_{1bc} , i.e.,

$$\begin{aligned}
I &\geq I_{sp} \\
I_{sp} &= \frac{V}{N(2\pi)^D} \int_{V_{sp}} d^D k \frac{1}{|b\mathcal{S}_{\mathbf{Q}}(T, b)| + \mathbf{k}^2 X} \\
&= \frac{V\Omega_D}{N(2\pi)^D} \int_0^{k_0} dk \frac{k^{D-1}}{|b\mathcal{S}_{\mathbf{Q}}(T, b)| + \mathbf{k}^2 X} \\
&= \frac{const}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|} \int_0^{k_0} \frac{dk}{k} \underbrace{\frac{k^D}{1 + \mathbf{k}^2 \frac{X}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|}}}_{:=x^2} \\
&= \frac{const}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|} \left(\frac{|b\mathcal{S}_{\mathbf{Q}}(T, b)|}{X} \right)^{D/2} \int_0^{k_0 \sqrt{\frac{X}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|}}} \frac{dx}{x} \frac{x^D}{1 + x^2} \\
&= const |b\mathcal{S}_{\mathbf{Q}}(T, b)|^{\frac{D-2}{2}} \int_0^{k_0 \sqrt{\frac{X}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|}}} \frac{dx}{x} \frac{x^D}{1 + x^2} .
\end{aligned}$$

So finally we have

$$S(S+1) \geq const k_B T \frac{\mathcal{S}_{\mathbf{Q}}^2(T, b)}{\hbar^2} |b\mathcal{S}_{\mathbf{Q}}(T, b)|^{\frac{D-2}{2}} \int_0^{k_0 \sqrt{\frac{X}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|}}} \frac{dx}{x} \frac{x^D}{1 + x^2} ,$$

or alternative

$$1 \geq const \cdot T \cdot \left| \mathcal{S}_{\mathbf{Q}}(T, b) \right|^{\frac{D+2}{2}} |b|^{\frac{D-2}{2}} \underbrace{\int_0^{k_0 \sqrt{\frac{X}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|}}} \frac{dx}{x} \frac{x^D}{1 + x^2}}_{=K_D} . \quad (6.65)$$

We are interested in the spontaneous magnetization $b \rightarrow 0$, i.e. the upper integration limit goes to ∞ .

1D

In the 1D case, the integral for $b \rightarrow 0$ becomes

$$K_1 = \int_0^{k_0 \sqrt{\frac{X}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|}}} dx \frac{1}{1 + x^2} \xrightarrow{b \rightarrow 0} \int_0^{\infty} dx \frac{1}{1 + x^2} = \frac{\pi}{2}$$

Hence

$$\begin{aligned} 1 &\geq \text{const } T \left(\mathcal{S}_{\mathbf{Q}}(T, b) \right)^{\frac{3}{2}} |b|^{-\frac{1}{2}} \\ \frac{|b|}{T^2} &\geq \text{const} \left(\mathcal{S}_{\mathbf{Q}}(T, b) \right)^3 \\ \mathcal{S}_{\mathbf{Q}}(T, b) &\leq \left(\frac{|b|}{T^2} \right)^{1/3}. \end{aligned}$$

For finite temperature, the rhs tends to zero for $b \rightarrow 0$. Hence for 1D and finite T

$$\lim_{b \rightarrow 0} \mathcal{S}_{\mathbf{Q}}(T, b) = 0, \quad (6.66)$$

i.e. there is no spontaneous magnetization, irrespective of \mathbf{Q} , for finite T . **The inequality does not rule out a finite spontaneous magnetization for $T = 0$.**

2D

In the 2D case, the integral K_D is a bit more tricky as it diverges for $b \rightarrow 0$

$$\begin{aligned} K_2 &= \int_0^{k_0 \sqrt{\frac{X}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|}}} dx \frac{x}{1+x^2} \\ &= \frac{1}{2} \int_0^{\frac{k_0^2 X}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|}} dz \frac{1}{1+z} \\ &= \frac{1}{2} \ln \left(1 + \frac{k_0^2 X}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|} \right). \end{aligned}$$

For $b \rightarrow 0$ it behaves like

$$K_2 = \frac{1}{2} \ln \left(\frac{k_0^2 X}{|b\mathcal{S}_{\mathbf{Q}}(T, b)|} \right) = -\frac{1}{2} \ln \left(\frac{|b\mathcal{S}_{\mathbf{Q}}(T, b)|}{k_0^2 X} \right) = \frac{1}{2} |\ln(|b/b_0|)|,$$

where we have defined the positive parameter $b_0 = k_0^2 X / |\mathcal{S}_{\mathbf{Q}}(T, b)|$ and we have used that $b \rightarrow 0$ result in a negative logarithm. Then the inequality equation (6.65) [\[previous page\]](#) yields

$$\begin{aligned} 1 &\geq \frac{\text{const}}{2} T \left(\mathcal{S}_{\mathbf{Q}}(T, b) \right)^2 |b|^0 |\ln(|b/b_0|)| \\ \left(\mathcal{S}_{\mathbf{Q}}(T, b) \right)^2 &\leq \frac{\text{const}}{T |\ln(|b/b_0|)|}. \end{aligned}$$

The story is the same as in 1D. The rhs goes to zero for $b \rightarrow 0$ and finite T . **Nothing can be said about $T = 0$.**

3D

Eventually in the 3D case, the integral K_D yields

$$\begin{aligned}
 K_3 &= \int_0^{k_0 \sqrt{\frac{X}{|b\mathcal{S}_{\mathbf{Q}}(T,b)|}}} dx \frac{x^2}{1+x^2} \\
 &= \int_0^{k_0 \sqrt{\frac{X}{|b\mathcal{S}_{\mathbf{Q}}(T,b)|}}} dx \left(1 - \frac{1}{1+x^2}\right) \\
 &= \sqrt{\frac{c}{|b\mathcal{S}_{\mathbf{Q}}(T,b)|}} - \underbrace{K_{1D}}_{=\pi/2}
 \end{aligned}$$

Inserting in the inequality equation (6.65) [p. 165] yields

$$\begin{aligned}
 1 &\geq \text{const } T \left(\mathcal{S}_{\mathbf{Q}}(T,b) \right)^{\frac{5}{2}} |b|^{\frac{1}{2}} \left(\frac{c}{\sqrt{|b\mathcal{S}_{\mathbf{Q}}(T,b)|}} - \frac{\pi}{2} \right) \\
 &\geq \text{const } T \left(\mathcal{S}_{\mathbf{Q}}(T,b) \right)^2 \\
 \left(\mathcal{S}_{\mathbf{Q}}(T,b) \right)^2 &\leq \frac{\text{const}}{T}
 \end{aligned}$$

In this case we do not obtain a useful inequality. In other words, the Mermin-Wagner theorem does not rule out spontaneous magnetization for finite T in 3D.

6.5.4 Exact ground-state of the ferromagnetic Heisenberg model

Here we consider only the isotropic ferromagnetic ($J_{jj'} > 0$) Heisenberg model with a homogenous magnetic field pointing in the z -direction. We readily see that the ground state is given by the state, where all spins are maximally aligned in the negative z -direction

$$|0\rangle = \otimes_{j=1}^N | -S \rangle_j \quad (6.67)$$

with

$$S_j^z |m\rangle_j = \hbar m |m\rangle_j \quad (6.68a)$$

$$S_j^2 |m\rangle_j = \hbar^2 S(S+1) |m\rangle_j. \quad (6.68b)$$

Applying the hamiltonian to $|0\rangle$ yields

$$\begin{aligned}
H|0\rangle &= - \sum_{jj'} J_{jj'} S_j^z S_{j'}^z |0\rangle - \sum_{jj'} J_{jj'} S_j^+ \underbrace{S_{j'}^- |0\rangle}_{=0} + b \sum_j S_j^z |0\rangle \\
&= - \sum_{jj'} J_{jj'} \hbar^2 S^2 |0\rangle - b \sum_j \hbar S |0\rangle \\
&= -\hbar \left(N \sum_l J(|\mathbf{R}_l|) \hbar S^2 + b \sum_j S \right) |0\rangle \\
&= -\hbar N \left(\hbar \tilde{J}(0) S^2 + b S \right) |0\rangle \\
\tilde{J}(0) &= \sum_l J(|\mathbf{R}_l|) .
\end{aligned}$$

We have introduced the Fourier transform of the exchange coupling.

$$\tilde{J}(\mathbf{k}) = \sum_l J(|\mathbf{R}_l|) e^{i\mathbf{k}\mathbf{R}_l} . \quad (6.69)$$

Obviously, $|0\rangle$ is an eigenvector. We consider

$$\begin{aligned}
(\mathbf{S}_j + \mathbf{S}_{j'})^2 &= \mathbf{S}_j^2 + \mathbf{S}_{j'}^2 + 2\mathbf{S}_j \mathbf{S}_{j'} \\
-\mathbf{S}_j \mathbf{S}_{j'} &= \frac{1}{2}(\mathbf{S}_j^2 + \mathbf{S}_{j'}^2) - \frac{1}{2}(\mathbf{S}_j + \mathbf{S}_{j'})^2
\end{aligned}$$

All spins have magnitude S . We consider an arbitrary vector $|\psi\rangle$, which is an eigenstate of all \mathbf{S}_j^2 with eigenvalue $S(S+1)$ but otherwise arbitrary. Then

$$-\langle \mathbf{S}_j \rangle \mathbf{S}_{j'} = S(S+1) - \frac{1}{2} \langle (\mathbf{S}_j + \mathbf{S}_{j'})^2 \rangle$$

Now $\mathbf{S}' := \mathbf{S}_j + \mathbf{S}_{j'}$ is an effective spin where the eigenvalues of \mathbf{S}'^2 are given bei $S'(S'+1)$ with $S' \in \hbar\{0, 1, \dots, 2S\}$. Consequently,

$$\frac{1}{2} \langle (\mathbf{S}_j + \mathbf{S}_{j'})^2 \rangle \leq 2S(2S+1) .$$

Then

$$-\langle \mathbf{S}_j \rangle \mathbf{S}_{j'} \geq S(S+1)S(2S+1) = S^2$$

Finally that means if $J_{jj'} \geq 0 \forall j, j'$

$$\begin{aligned}
\langle H_0 \rangle &= \sum_{jj'} J_{jj'} \left(-\langle \mathbf{S}_j \rangle \mathbf{S}_{j'} \right) \\
&\geq -S^2 \hbar^2 \sum_{jj'} J_{jj'} \\
\langle H_0 \rangle &\geq -N \hbar^2 \tilde{J}(0) .
\end{aligned}$$

For the Zeeman term we see readily

$$\langle H_Z \rangle \geq -bS\hbar$$

Hence in total we have for the energy

$$E \geq -N\hbar^2 \tilde{J}(0) - bS\hbar = E_0$$

Since there is no energy lower than the ferromagnetic state, it is the ground-state. Moreover, we see that

$$S_{total}^z = \sum_j \mathbf{S}_j^z |0\rangle = \hbar N S |0\rangle .$$

The groundstate is an eigenstate of S_{total}^z and also of

$$\begin{aligned} \mathbf{S}_{total}^2 &= \sum_{j \neq j'} \mathbf{S}_j \mathbf{S}_{j'} + \sum_j \mathbf{S}_j^2 \\ \mathbf{S}_{total}^2 |0\rangle &= \sum_{j \neq j'} \mathbf{S}_j \mathbf{S}_{j'} \mathbf{S}_{total}^2 |0\rangle + N\hbar^2 S(S+1) |0\rangle \\ \mathbf{S}_{total}^2 |0\rangle &= \sum_{j \neq j'} \hbar^2 S^2 |0\rangle + \underbrace{S_j^+ S_{j'}^-}_{=0} |0\rangle + NS(S+1)\hbar^2 |0\rangle \\ &= \left(N(N-1)\hbar^2 S^2 + NS(S+1)\hbar^2 \right) |0\rangle \\ &= \hbar^2 \left(N^2 S^2 - \cancel{NS^2} + \cancel{NS^2} + NS \right) |0\rangle \\ &= \hbar^2 NS(NS+1) |0\rangle \end{aligned}$$

So it $|0\rangle$ an eigenstate of \mathbf{S}_{total} with maximum magnitude $NS\hbar$.

6.5.5 Spin waves in the ferromagnetic Heisenberg model

Next we study the low-laying excited states. To this end we first consider the hamiltonian in Fourier space. The details of the Fourier transform as defined in equation (6.52) [p. 162] are

$$S_k^\alpha = \sum_j S_j^\alpha e^{i\mathbf{k}\mathbf{R}_j} , \quad \alpha \in \{x, y, z\} \quad (6.70a)$$

$$S_j^\alpha = \frac{1}{N} \sum_k S_k^\alpha e^{-i\mathbf{k}\mathbf{R}_j} \quad (6.70b)$$

We recall the commutation relations

$$[S_j^\alpha S_{j'}^\beta] = \delta_{jj'} i\hbar \varepsilon_{\alpha\beta\gamma} S_j^\gamma, \quad (6.71a)$$

$$[S_j^z S_{j'}^\pm] = \pm \delta_{jj'} \hbar S_j^\pm, \quad (6.71b)$$

$$[S_j^-, S_{j'}^+] = -2\hbar \delta_{jj'} S_j^z. \quad (6.71c)$$

Then

$$[S_{\mathbf{k}}^z S_{\mathbf{k}'}^\pm] = \pm \hbar S_{\mathbf{k}+\mathbf{k}'}^\pm, \quad (6.72a)$$

$$[S_{\mathbf{k}}^-, S_{\mathbf{k}'}^+] = -2\hbar S_{\mathbf{k}+\mathbf{k}'}^z \quad (6.72b)$$

Proof

$$\begin{aligned} [S_j^z S_{j'}^\pm] &= [S_j^z S_{j'}^x] \pm i [S_j^z S_{j'}^y] \\ &= \delta_{jj'} i\hbar \left(\varepsilon_{zxy} S_j^y \pm i \varepsilon_{zyx} S_j^x \right) \\ &= \delta_{jj'} \hbar \left(i \underbrace{\varepsilon_{zxy}}_{=+1} S_j^y \mp \underbrace{\varepsilon_{zyx}}_{=-1} S_j^x \right) \\ &= \delta_{jj'} \hbar \left(i S_j^y \pm S_j^x \right) \\ &= \pm \delta_{jj'} \hbar \left(S_j^x \pm i S_j^y \right). \end{aligned}$$

$$\begin{aligned} [S_{\mathbf{k}}^z S_{\mathbf{k}'}^\pm] &= \sum_{jj'} e^{i(\mathbf{k}\mathbf{x}_j + \mathbf{k}'\mathbf{x}_{j'})} [S_j^z S_{j'}^\pm] \\ &= \pm \hbar \sum_{jj'} e^{i(\mathbf{k}\mathbf{x}_j + \mathbf{k}'\mathbf{x}_{j'})} \delta_{jj'} S_j^\pm \\ &= \pm \hbar \sum_j e^{i(\mathbf{k}+\mathbf{k}')\mathbf{x}_j} S_j^\pm \\ &= \pm \hbar S_{\mathbf{k}+\mathbf{k}'}^\pm. \end{aligned}$$

$$\begin{aligned} [S_j^-, S_{j'}^+] &= [(S_j^x - iS_j^y), (S_{j'}^x + iS_{j'}^y)] \\ &= i[S_j^x, S_{j'}^y] - [S_j^y, S_{j'}^x] \\ &= 2i\delta_{jj'} (i\hbar S_j^z) \\ &= -2\hbar \delta_{jj'} S_j^z. \end{aligned}$$

$$\begin{aligned}
[S_{\mathbf{k}}^-, S_{\mathbf{k}'}^+] &= \sum_{jj'} e^{i(\mathbf{k}\mathbf{x}_j + \mathbf{k}'\mathbf{x}_{j'})} \underbrace{[S_j^-, S_{j'}^+]}_{=-2\hbar\delta_{jj'}S_j^z} \\
&= -2\hbar \sum_j e^{i(\mathbf{k}+\mathbf{k}')\mathbf{x}_j} S_j^z \\
&= -2\hbar S_{\mathbf{k}+\mathbf{k}'}^z
\end{aligned}$$

q.e.d. ✓

and obtain

$$\begin{aligned}
H &= - \sum_{jj'} J_{jj'} \left(S_j^z S_{j'}^z + S_j^+ S_{j'}^- \right) + b \sum_j S_j^z \\
&= - \frac{1}{N^2} \sum_{kk'} \sum_{jj'} J \underbrace{(j' - j)}_{=l} e^{-i(\mathbf{R}_j \mathbf{k} + \mathbf{R}_{j'} \mathbf{k}')} \left(S_k^z S_{k'}^z + S_k^+ S_{k'}^- \right) \\
&\quad + b \frac{1}{N} \sum_k \underbrace{\sum_j e^{i\mathbf{R}_j \mathbf{k}} S_k^z}_{=N\delta_{\mathbf{k},0}} \\
&= - \frac{1}{N^2} \sum_{kk'} \sum_{jl} J(|\mathbf{R}_l|) e^{-i(\mathbf{R}_j \mathbf{k} + (\mathbf{R}_j + \mathbf{R}_l) \mathbf{k}')} \left(S_k^z S_{k'}^z + S_k^+ S_{k'}^- \right) + b S_{\mathbf{k}=0}^z \\
&= - \frac{1}{N} \sum_{kk'} \sum_l J(|\mathbf{R}_l|) e^{-i\mathbf{k}' \mathbf{R}_l} \underbrace{\sum_j e^{-i\mathbf{R}_j (\mathbf{k} + \mathbf{k}')}}_{=N\delta_{\mathbf{k}', -\mathbf{k}}} \left(S_k^z S_{k'}^z + S_k^+ S_{k'}^- \right) + b S_{\mathbf{k}=0}^z .
\end{aligned}$$

Eventually, we have with equation (6.69) [p. 168]

$$H = - \frac{1}{N} \sum_k \tilde{J}(k) \left(S_k^z S_{-k}^z + S_k^+ S_{-k}^- \right) + b S_{\mathbf{k}=0}^z . \quad (6.73)$$

There exist exact eigenstates for the low-lying excitations given by

$$|\tilde{\psi}(q)\rangle = S_q^+ |0\rangle . \quad (6.74)$$

First we will prove that these states are indeed eigenstates

$$\begin{aligned}
H|\tilde{\psi}(q)\rangle &= H S_q^+ |0\rangle \\
&= S_q^+ \underbrace{H|0\rangle}_{=E_0|0\rangle} + [H, S_q^+] |0\rangle
\end{aligned}$$

So far we have

$$H|\tilde{\psi}(q)\rangle = E_0|\tilde{\psi}(q)\rangle + [H, S_q^+]|0\rangle .$$

For the commutator we first evaluate the Zeeman part of the hamiltonian

$$\begin{aligned} [H_Z, S_q^+] &= b[S_{q=0}^z, S_q^+] = b\hbar S_{q+0}^+ \\ [H_Z, S_q^+]|0\rangle &= \hbar b S_q^+|0\rangle = \hbar b|\tilde{\psi}(q)\rangle . \end{aligned}$$

For the Heisenberg part of the hamiltonian we obtain

$$\begin{aligned} [H_H, S_q^+] &= -\frac{1}{N} \sum_k \tilde{J}(k) \left([S_k^z S_{-k}^z, S_q^+] + [S_k^+ S_{-k}^-, S_q^+] \right) \\ &= -\frac{1}{N} \sum_k \tilde{J}(k) \left(S_k^z [S_{-k}^z, S_q^+] + [S_k^z, S_q^+] S_{-k}^z + S_k^+ [S_{-k}^-, S_q^+] \right) \\ &= -\frac{\hbar}{N} \sum_k \tilde{J}(k) \left(\underbrace{S_k^z S_{q-k}^+}_{=S_{q-k}^+ S_k^z + [S_k^z, S_{q-k}^+]} + S_{q+k}^+ S_{-k}^z - 2S_k^+ S_{q-k}^z \right) \\ &\quad \underbrace{= \hbar S_q^+}_{\text{blue}} \\ &= -\frac{\hbar}{N} \sum_k \tilde{J}(k) \left(S_{q-k}^+ S_k^z + S_{q+k}^+ S_{-k}^z - 2S_k^+ S_{q-k}^z \right) - \frac{\hbar^2}{N} \sum_k \tilde{J}(k) S_q^+ . \end{aligned}$$

The last term vanishes because

$$\sum_k \tilde{J}(\mathbf{k}) = \sum_l J(|\mathbf{R}_l|) \underbrace{\sum_k e^{i\mathbf{k}\mathbf{R}_l}}_{=N\delta_{l,0}} = N J_l = 0 .$$

We also have

$$\begin{aligned} J_k^z|0\rangle &= \sum_l e^{i\mathbf{k}\mathbf{R}_l} \underbrace{S_l^z|0\rangle}_{=-\hbar S|0\rangle} \\ &= -\hbar S \left(\sum_l e^{i\mathbf{k}\mathbf{R}_l} \right) |0\rangle \\ &= -\hbar S N \delta_{k,0} |0\rangle . \end{aligned}$$

Hence

$$\begin{aligned} [H_H, S_q^+]|0\rangle &= \frac{\hbar^2 S N}{N} \sum_{\mathbf{k}} \tilde{J}(\mathbf{k}) \left(S_{\mathbf{q}-\mathbf{k}}^+ \delta_{\mathbf{k},0} + S_{\mathbf{q}+\mathbf{k}}^+ \delta_{\mathbf{k},0} - 2S_{\mathbf{k}}^+ \delta_{\mathbf{k}-\mathbf{q}} \right) |0\rangle \\ &= \hbar^2 S N \frac{\hbar}{N} \left(2\tilde{J}(0) - 2\tilde{J}(q) \right) S_q^+ |0\rangle \\ &= 2\hbar^2 S (\tilde{J}(0) - \tilde{J}(q)) |\tilde{\Psi}(q)\rangle \end{aligned}$$

Moreover, the field term contributes

$$[H_b, S_{\mathbf{q}}^+] = b[S_{\mathbf{k}=0}^z, S_{\mathbf{q}}^+] = b\hbar S_{\mathbf{q}}^+$$

Putting all terms together proves that $|\tilde{\psi}(q)\rangle$ is an eigen vector

$$H|\tilde{\Psi}(q)\rangle = (E_0 + \hbar\omega_q)|\tilde{\Psi}(q)\rangle, \quad (6.75)$$

with eigenvalue

$$\omega_q = b + 2S(\tilde{J}(0) - \tilde{J}(q)). \quad (6.76)$$

For nearest neighbour exchange interactions,

$$\tilde{J}(q) = J \sum_{\delta} e^{i\delta\mathbf{q}} = 2J \sum_{\nu=1}^D \cos(q_{\nu}),$$

The sum runs over the cartesian coordinates. Hence

$$\tilde{J}(0) - \tilde{J}(q) = 2J \sum_{\nu} (1 - \cos(q_{\nu})).$$

For $b = 0$ and small values of q_{α} the leading order of the Taylor expansion yields

$$\hbar\omega_q = 2\hbar S(\tilde{J}(0) - \tilde{J}(q)) = D\mathbf{q}^2.$$

The excitation has a quadratic dispersion with a *spin wave stiffness* $D = 2\hbar S J$. The excitation energy tends continuously to zero for small q . This is a typical feature of a *Goldstone mode*, which tries to restore the broken symmetry.

We will study further properties of the one-magnon excitation. We start out with the scalar product of one-magnon states with different wavevectors

$$\begin{aligned} \langle \tilde{\Psi}(q) | \tilde{\Psi}(q') \rangle &= \langle 0 | S_{-q}^- S_{q'}^+ | 0 \rangle \\ &= \langle 0 | S_{q'}^+ \underbrace{S_{-q}^-}_{=0} | 0 \rangle + \langle 0 | [S_{-q}^-, S_{q'}^+] | 0 \rangle \\ &= -2\hbar \langle 0 | \underbrace{S_{q'-q}^z}_{=\delta_{q,q'}(-SN\hbar)} | 0 \rangle \\ &= \delta_{q,q'} 2SN\hbar^2. \end{aligned}$$

We have used

$$\begin{aligned}
 S_q^z |0\rangle &= \sum_l e^{i\mathbf{R}_l \mathbf{q}} \underbrace{S_l^z |0\rangle}_{=-S\hbar|0\rangle} \\
 &= -S\hbar \left(\underbrace{\sum_l e^{i\mathbf{R}_l \mathbf{q}}}_{=N\delta_{q,0}} \right) |0\rangle \\
 &= -SN\hbar\delta_{q,0} |0\rangle .
 \end{aligned}$$

q.e.d. ✓

The one-magnon states are orthogonal and the correctly normalized vectors are

ONE-MAGNON STATES		
eigenvector:	$ \psi(\mathbf{q})\rangle = \frac{1}{\hbar\sqrt{2NS}} S_q^+ 0\rangle .$	(6.77a)
excitation energy:	$\omega_q = b + 2S(\tilde{J}(0) - \tilde{J}(q))$	(6.77b)

Properties of the single magnon state

The one-magnon vectors are also eigenvectors of

$$S_{total}^z = \sum_l S_l^z = S_{q=0}^z .$$

The prove is as follows

$$\begin{aligned}
 S_{q=0}^z S_q^+ |0\rangle &= S_q^+ \underbrace{S_{q=0}^z |0\rangle}_{=-SN\hbar|0\rangle} + \underbrace{[S_{q=0}^z, S_q^+]}_{=\hbar S_{q+0}^+} |0\rangle \\
 &= \hbar(-NS + 1) S_q^+ |0\rangle
 \end{aligned}$$

The eigenvalue of S_{total}^z has been changed by $+\hbar$. Now it is interesting to compare that with the expectation value of S_j^z of the spin at site \mathbf{R}_j

$$\langle \psi(\mathbf{q}) | S_j^z | \psi(\mathbf{q}) \rangle = \frac{1}{N} \sum_k e^{-i\mathbf{k}\mathbf{R}_j} \langle \psi(\mathbf{q}) | S_k^z | \psi(\mathbf{q}) \rangle . \quad (6.78)$$

We need

$$\begin{aligned} \langle 0 | S_{-q}^- S_k^z S_q^+ | 0 \rangle &= \langle 0 | S_{-q}^- S_q^+ \underbrace{S_k^z | 0 \rangle}_{=-NS\hbar\delta_{k,0}|0\rangle} + \langle 0 | S_{-q}^- [S_k^z S_q^+] | 0 \rangle \\ a &= -SN\hbar\delta_{k,0} \underbrace{\langle 0 | S_{-q}^- S_q^+ | 0 \rangle}_{=2SN\hbar^2} + \hbar \underbrace{\langle 0 | S_{-q}^- S_{k+q}^+ | 0 \rangle}_{=2SN\hbar\delta_{\mathbf{k}}} \\ &= 2SN\hbar^2\delta_{\mathbf{k},0}(-SN+1) . \end{aligned}$$

We recall that the normalization one the one-magnon states is given by $\langle 0 | S_{-q}^- S_q^+ | 0 \rangle = 2NS\hbar^2$. Hence

$$\langle S_{\mathbf{k}}^z \rangle = \frac{\langle 0 | S_{-\mathbf{q}}^- S_{\mathbf{k}}^z S_{\mathbf{q}}^+ | 0 \rangle}{\langle 0 | S_{-q}^- S_q^+ | 0 \rangle} = \delta_{k,0} \hbar \left(-SN + 1 \right) .$$

Inserting in equation (6.78) yields

$$\langle \psi(\mathbf{q}) | S_j^z | \psi(\mathbf{q}) \rangle = -\hbar \left(S - \frac{1}{N} \right) \sum_k e^{-i\mathbf{k}\mathbf{R}_j} \delta_{k,0} = -\hbar S + \frac{\hbar}{N} .$$

The value of S_j^z is increased by \hbar/N at each site, irrespective of the index j .

6.5.6 Mean field approximation of the isotropic Heisenberg model

The derivation of the MFA results is very similar to that in the Ising model. The hamiltonian in MFA for an homogeneous magnetic field

$$H^{\text{MFA}} = -\frac{1}{2} \sum_{jj'} J_{jj'} (\langle \mathbf{S}_j \rangle \mathbf{S}_{j'} + \mathbf{S}_j \langle \mathbf{S}_{j'} \rangle) + \frac{1}{2} \sum_{jj'} J_{jj'} \langle \mathbf{S}_j \rangle \langle \mathbf{S}_{j'} \rangle - \mathbf{b} \sum_j \mathbf{S}_j \quad (6.79)$$

We consider only the restricted MFA, where we retain the translational symmetry of the hamiltonian, i.e.

$$\langle \mathbf{S}_j \rangle = \mathcal{S} \quad \forall j$$

Then

$$\begin{aligned}
 H^{\text{MFA}} &= -J \left(\underbrace{\sum_{j'} J_{jj'}}_{=\tilde{J}(0)} \right) \mathbf{S} \sum_j \mathbf{S}_j + \mathbf{S}^2 \frac{1}{2} \underbrace{\sum_{jj'} J_{jj'}}_{=N\tilde{J}(0)} - \mathbf{b} \sum_j \mathbf{S}_j \\
 &= -(\tilde{J}(0) \mathbf{S} + \mathbf{b}) \sum_j \mathbf{S}_j + \frac{N\tilde{J}(0)}{2} \mathbf{S}^2 .
 \end{aligned}$$

We have employed equation (6.69) [p. 168]. It is obvious in an isotropic model to assume that the mean field will point into the same direction as the external field. Without loss of generality, we assume that the external field defines the z -direction ($\mathbf{b} = b\mathbf{e}_z$). With $\mathcal{S} = \langle S_i^z \rangle$

$$H^{\text{MFA}} = - \underbrace{(\tilde{J}(0) \mathcal{S} + b)}_{=b'} \sum_j S_j^z + \frac{N\tilde{J}(0)}{2} \mathcal{S}^2 ,$$

where S_j^z is an operator $S = \langle S_i^z \rangle$. The partition function is readily computed in the eigen basis of the S_i^z operators.

Since the spins are no longer interacting and the effective field b' is translational invariant, the partition function of N spins Z_N is simply the N -th power of Z_1 , or rather (see also equation (1.7) [p. 10] of the Ising model)

$$\begin{aligned}
 \ln(Z_N) &= N \ln(Z_1) \\
 Z_1 &= e^{-\frac{\beta\tilde{J}(0)}{2}\mathcal{S}^2} \sum_{\sigma=-S}^S e^{h'\sigma} \\
 &= e^{-\frac{\beta\tilde{J}(0)}{2}\mathcal{S}^2} e^{-Sh'} \sum_{\sigma=0}^{2S} e^{h'\sigma} \\
 &= e^{-\frac{\beta\tilde{J}(0)}{2}\mathcal{S}^2} e^{-Sh'} \frac{e^{h'(2S+1)} - 1}{e^{h'} - 1} y \\
 &= e^{-\frac{\beta\tilde{J}(0)}{2}\mathcal{S}^2} \frac{\sinh(h'(2S+1)/2)}{\sinh(h'/2)}
 \end{aligned}$$

with $h' = \beta b'$. Hence

$$\frac{\ln(Z_N)}{N} = -\beta \frac{\tilde{J}(0)}{2} \mathcal{S}^2 + \ln [\sinh(h'(2S+1)/2)] - \ln [\sinh(h'/2)]$$

and for the free energy $\frac{F}{N} = -k_B T \frac{\ln(Z_N)}{N}$ we obtain

FREE ENERGY OF THE ISOTROPIC HEISENBERG MODEL
(in mean-field approximation)

$$\frac{F}{N} = \frac{\tilde{J}(0)\mathcal{S}^2}{2} - k_B T \left(\ln [\sinh (h'(2S+1)/2)] - \ln [\sinh (h'/2)] \right) \quad (6.80)$$

Like in the Ising case, the most simply way to compute the order parameter \mathcal{S} is via

$$\begin{aligned} \mathcal{S} &= \frac{1}{N} \frac{d}{dh'} \ln(Z) = \frac{d}{dh'} \left(\ln [\sinh (h'(2S+1)/2)] - \ln [\sinh (h'/2)] \right) \\ &= \frac{2S+1}{2} \coth (h'(2S+1)/2) - \frac{1}{2} \coth (h'/2) . \end{aligned}$$

In terms of the Brillouin function, defined in equation (6.17) [p. 146], we have

ORDER PARAMETER OF THE ISOTROPIC HEISENBERG MODEL
(in mean-field approximation)

$$\frac{\mathcal{S}}{S} = \mathcal{B}_S(Sh') \quad (6.81a)$$

$$h' = \beta(\tilde{J}(0)\mathcal{S} + b) . \quad (6.81b)$$

For $S = 1/2$ we obtain according to equation (6.22) [p. 148]

$$2\mathcal{S} = \mathcal{B}_{1/2}\left(\frac{h'}{2}\right) = \tanh\left(\frac{h'}{2}\right) . \quad (6.82)$$

This result agrees with that of the MFA result in equation (1.12) [p. 11] for the nn Ising model, if we take into account

$$\tilde{J}(0) = \sum_l J(|\mathbf{R}_l|) = zJ .$$

Then equation (6.82) becomes

$$2\mathcal{S} = \tanh\left(\beta\left(\frac{zJ}{4}2\mathcal{S} + \frac{b}{2}\right)\right) . \quad (6.83)$$

We also have to take into account for the spin-1/2 case

$$H_H^{\text{MFA}} = -\tilde{J}_H(0)\langle S_1 \rangle \sum_i S_i^z - b_H \sum_j S_j$$

If the spin eigenvalues are $S_i = \frac{1}{2}\sigma_i$, with $\sigma_i = \pm 1$ then

$$H_H^{\text{MFA}} = -\frac{\tilde{J}_H(0)}{4}\langle \sigma_1 \rangle \sum_i \sigma_i^z - \frac{b_H}{2} \sum_j \sigma_j$$

So we have the following relations between the Heisenberg- and the Ising parameters

$$J_I = \frac{J_H}{4}, \quad b_I = \frac{b_H}{2}.$$

With these parameters equation (6.83) [\[previous page\]](#) turns into

$$\langle \sigma_1 \rangle = \tanh \left(\beta (z J_I \langle \sigma_1 \rangle + b_I) \right).$$

which is identical to that of the Ising model equation (1.12) [\[p. 11\]](#).

6.5.7 Curie temperature

According to equation (6.20) [\[p. 147\]](#) the equation for the order parameter without external field reads for $T \leq T_C$

$$\begin{aligned} \frac{S}{S} &= \mathcal{B}_S \left(\underbrace{\beta \tilde{J}(0) S^2}_{=\alpha} \underbrace{\frac{S}{S}}_{=x} \right) \\ x &= \frac{S+1}{3S} \alpha x - \underbrace{\frac{2S^3 + 4S^2 + 3S + 1}{90S^3} \alpha^3 x^3}_{=D}. \end{aligned}$$

Removing the trivial solution ($x = 0$) we are left with

$$\begin{aligned} Dx^2 &= \left(\frac{S+1}{3S} \alpha - 1 \right) \\ x &\propto \left(\frac{S(S+1)}{3} \tilde{J}(0) \beta - 1 \right)^{1/2}. \end{aligned}$$

There is a temperature (Curie temperature), at which x goes to zero. The condition for it yields

$$k_B T_C = \tilde{J}(0) \frac{S(S+1)}{2}. \quad (6.84)$$

Then the order parameter slightly below T_C can also be written as

$$x \propto \left(\frac{T_C}{T} - 1 \right) \simeq \varepsilon^{1/2} .$$

Hence the critical exponent for the order parameter is again $\beta = 1/2$.

6.5.8 Internal energy

Like in the Ising case we obtain for the internal energy

$$U = \langle H^{MFA} = -\frac{N\tilde{J}(0)}{2} \mathcal{S}^2 \rangle, \quad (6.85)$$

which is zero above T_C and slightly below T_C it has the form

$$\frac{U}{N} = \frac{\tilde{J}(0)}{2D} (T - T_C) ,$$

resulting in a specific heat close to T_C

$$\frac{C}{N} = \begin{cases} \frac{\tilde{J}(0)}{2D} > 0 & \text{for } T < T_C \\ 0 & \text{for } T > T_C . \end{cases}$$

Like in the Ising case there is a discontinuous jump the the specific heat, but no power law behaviour

6.5.9 Magnetic susceptibility

$$\chi = \mu_0 \left. \frac{\partial M}{\partial h} \right|_T \Big|_{h=0}$$

Since the equation has the same structure as in the Ising case, we again find

$$\chi \simeq A_{\pm} |\varepsilon|^{-\gamma_{\pm}}$$

with $A_+ = 2A_-$ and $\gamma_+ = \gamma_- = 1$.

Chapter 7

Non-equilibrium physics

7.1 Boltzmann Equation

7.2 Stochastic Method

7.2.1 Brownian motion

We consider the irregular motion of particles caused by the random scatter by much smaller particles. The latter form a fluid, in which the bigger particle moves. The eom therefore reads

LANGEVIN EQUATION	
$m \frac{d}{dt} \mathbf{v} = -\alpha \mathbf{v} + \mathbf{F}(t) ,$	(7.1)

The first term on the rhs describes the friction (Newtonian fluid) and the last term the stochastic (random) force due to the collisions of the light particles. It is assumed to be independent of velocity and fluctuating on small times scale, compared to the time scale typical for the heavy particle. For simplicity we consider only 1D motion and introduce

$$\frac{d}{dt} v + \gamma v = \mathbf{A}(t) , \quad (7.2)$$

where $\lambda = \alpha/m$ and $A(t) = F(t)/m$. The homogeneous equation has the solution

$$v(t) = v_0 e^{-\gamma t} , .$$

For the inhomogeneous equation we use the ansatz

$$v(t) = v_0(t) e^{-\gamma t} , .$$

Insertion into the equation (7.2) yields

$$\begin{aligned} \dot{v}(t) &= -\gamma \underbrace{v_0(t) e^{-\gamma t}}_{=v(t)} + \dot{v}_0(t) e^{-\gamma t} \stackrel{!}{=} -\gamma v(t) + A(t) \\ \Rightarrow \quad \dot{v}_0(t) &= e^{\gamma t} A(t) . \\ \text{with} \quad v_0(0) &= v_0 . \end{aligned}$$

Integration yields

$$v_0(t) = v_0 + \int_0^t e^{t'\gamma} A(t') dt' .$$

In total we have

$$v(t) = v_0 e^{-\gamma t} + \int_0^t e^{-\gamma(t-t')} A(t') dt' . \quad (7.3)$$

This is the solution of a particular for one particular realization of the stochastic force $A(t)$. As a matter of fact, we are interested in the pdf $p_t(v|v_0)$, that the particle has a velocity in the interval $(v, v+dv)$ at time t . For sufficiently long time, we assume that we will recover the Maxwell-Boltzmann velocity distribution, i.e.

$$p_t(v|v_0) \xrightarrow[t \rightarrow \infty]{} \left(\frac{m}{2\pi k_B T} \right)^{1/2} e^{-\frac{mv^2}{2k_B T}} . \quad (7.4)$$

We can compute the mean

$$\langle v(t) \rangle = \int dv v p_t(v|v_0)$$

via the pdf or directly by averaging equation (7.5) , resulting in

$$\langle v(t) \rangle = v_0 e^{-\gamma t} + \int_0^t e^{-\gamma(t-t')} \langle A(t') \rangle dt' . \quad (7.5)$$

It is to be expected that stochastic force has zero mean, hence $\langle v(t) \rangle = 0$. Hence, there is an exponentially decreasing mean velocity for a given initial velocity v_0 .

$$\langle v(t) \rangle = v_0 e^{-\gamma t} .$$

Next we compute the variance of the velocity

$$\begin{aligned} \langle (v(t) - \langle v(t) \rangle)^2 \rangle &= \left\langle \left(\int_0^t e^{-\gamma(t-t')} (A(t') - \langle A(t') \rangle) dt' \right)^2 \right\rangle \\ &= \int_0^t dt' \int_0^t dt'' e^{-\gamma(t-t')} e^{-\gamma(t-t'')} \langle A(t') A(t'') \rangle . \end{aligned}$$

Finally we assume that the stochastic forces for different times are uncorrelated and homogeneous in time, i.e.

$$\langle A(t') A(t'') \rangle = \tau \delta(t' - t'') . \quad (7.6)$$

Then

$$\left\langle \left(v(t) - \langle v(t) \rangle \right)^2 \right\rangle = \tau \int_0^t dt' e^{-2\gamma(t-t')} = \frac{\tau}{2\gamma} (1 - e^{-2\gamma t}) \xrightarrow{t \rightarrow \infty} \frac{\tau}{2\gamma} .$$

According to our initial assumption that the pdf approaches the Maxwell-Boltzmann distribution in the long run, which has $\left\langle (\Delta v)^2 \right\rangle = \frac{k_B T}{m}$ (see equation (7.4)). Hence

$$\tau = \frac{2\gamma k_B T}{m} . \quad (7.7)$$

The variance of the velocity for finite times is then given by

$$\sigma^2(t) := \left\langle \left(v(t) - \langle v(t) \rangle \right)^2 \right\rangle = \frac{k_B T}{m} (1 - e^{-2\gamma t}) .$$

If the first moments 0 – 2 is the only (reliable) information about the pdf, then MaxEnt yields that it has to be Gaussian, with these moments, i.e.

$$p_t(v|v_0) = \frac{1}{\sqrt{2\pi\sigma^2(t)}} e^{-\frac{(v - \langle v(t) \rangle)^2}{2\sigma^2(t)}} \quad (7.8)$$

$$\langle v(t) \rangle = v_0 e^{-\gamma t} . \quad (7.9)$$

Chapter 8

Appendix

8.1 Sommerfeld expansion

We are interested in integrals of the form

$$I = \int_0^\infty f(\varepsilon) n_F(\varepsilon|\mu, T) d\varepsilon$$

for low temperatures. The function $f(\varepsilon)$ is assumed to be independent of T and regular at $\varepsilon = \mu$. First we split the integral as follows

$$I = \int_0^\mu f(\varepsilon) \frac{1}{e^{\beta(\varepsilon-\mu)} + 1} d\varepsilon + \int_\mu^\infty f(\varepsilon) \frac{1}{e^{\beta(\varepsilon-\mu)} + 1} d\varepsilon ,$$

and modify the first term using $1/(e^x + 1) = 1 - 1/(e^{-x} + 1)$

$$I = \underbrace{\int_0^\mu f(\varepsilon) d\varepsilon}_{=I_1} - \underbrace{\int_0^\mu f(\varepsilon) \frac{1}{e^{-\beta(\varepsilon-\mu)} + 1} d\varepsilon}_{=I_2} + \underbrace{\int_\mu^\infty f(\varepsilon) \frac{1}{e^{\beta(\varepsilon-\mu)} + 1} d\varepsilon}_{=I_3}$$

In I_2 we use the transformation

$$\begin{aligned} x &= -\beta(\varepsilon - \mu) , \\ \varepsilon &= \mu - k_B T x , \\ d\varepsilon &= -k_B T dx , \end{aligned}$$

and find

$$I_2 = -k_B T \int_0^{\beta\mu} \frac{f(\mu - k_B T x)}{e^x + 1} .$$

The kernel $1/(e^x - 1)$ decreases rapidly with x ; and for small values of T the upper integration limit $\beta\mu$ is much greater than 1, so we can as well extend the integral all the way up to infinity

$$I_2 = -k_B T \int_0^\infty \frac{f(\mu - k_B T x)}{e^x + 1} dx.$$

For I_3 we introduce the substitution

$$\begin{aligned} x &= \beta(\varepsilon - \mu), \\ \varepsilon &= \mu + k_B T x, \\ d\varepsilon &= k_B T dx, \end{aligned}$$

and obtain

$$I_3 = k_B T \int_0^\infty \frac{f(\mu + k_B T x)}{e^x + 1} dx.$$

Since $1/(e^x + 1)$ decreases rapidly, x is essentially restricted to $x \lesssim 1$. Hence $k_B T x \lesssim k_B T$. So if $k_B T/\mu$ is small, then we can use a Taylor expansion

$$f(\mu + s k_B T x) = \sum_{n=0}^{\infty} s^n \frac{(k_B T x)^n}{n!} f^{(n)}(\mu).$$

We need

$$\begin{aligned} I_3 - I_2 &= k_B T \int_0^\infty dx \left(f(\mu + k_B T x) - f(\mu - k_B T x) \right) \frac{1}{e^x + 1} \\ &= 2 \sum_{n=1}^{\text{odd}} \frac{(k_B T)^{n+1}}{n!} f^{(n)}(\mu) \int_0^\infty dx \frac{x^n}{e^x + 1} \\ &= 2 \sum_{n=1}^{\text{odd}} \frac{(k_B T)^{n+1}}{n!} f^{(n)}(\mu) \left(1 - \frac{1}{2^n}\right) \Gamma(n+1) \zeta(n+1). \end{aligned}$$

The final result reads

SOMMERFELD EXPANSION
$\int_0^\infty f(\varepsilon) n_F(\varepsilon \mu, T) d\varepsilon = \int_0^\mu f(\varepsilon) d\varepsilon + 2 \sum_{n=1}^{\text{odd}} \left(1 - \frac{1}{2^n}\right) \zeta(n+1) (k_B T)^{n+1} f^{(n)}(\mu) \quad (8.1)$

So the leading order terms in the Sommerfeld expansion are

$$I = \int_0^\mu f(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 f'(\mu) + \mathcal{O}\left(\left(\frac{k_B T}{\mu}\right)^4\right)$$

8.2 Euler Mac-Laurin formula

We are interested in sums of the form $\sum_{n=0}^\infty f(n + \frac{1}{2})$. We begin with the integral over $f(x)$, which shall be differentiable at least twice and the integral over $(0, \infty)$ shall exist. Then

$$\begin{aligned} \int_0^\infty f(x) dx &= \sum_{n=0}^\infty \int_n^{n+1} f(x) dx = \sum_{n=0}^\infty \int_{-\frac{1}{2}}^{\frac{1}{2}} f(n + \frac{1}{2} + \xi) d\xi \\ &= \sum_{n=0}^\infty \int_{-\frac{1}{2}}^{\frac{1}{2}} \left(f(n + \frac{1}{2}) + f'(n + \frac{1}{2})\xi + f''(n + \frac{1}{2})\frac{\xi^2}{2} + \dots \right) d\xi \\ &= \sum_{n=0}^\infty \left(f(n + \frac{1}{2}) \int_{-\frac{1}{2}}^{\frac{1}{2}} d\xi + f'(n + \frac{1}{2}) \int_{-\frac{1}{2}}^{\frac{1}{2}} \xi d\xi + \frac{f''(n + \frac{1}{2})}{2} \int_{-\frac{1}{2}}^{\frac{1}{2}} \xi^2 d\xi + \dots \right) d\xi \\ &= \sum_{n=0}^\infty \left(f(n + \frac{1}{2}) + f''(n + \frac{1}{2}) \frac{2}{2 \cdot 3 \cdot 2^3} + \dots \right) d\xi. \end{aligned}$$

The leading order terms are

$$\sum_{n=0}^\infty f(n + \frac{1}{2}) = \int_0^\infty f(x) dx - \frac{1}{24} \sum_{n=0}^\infty f''(n + \frac{1}{2}) + \dots$$

We can use this formula again to express the sum on the rhs also by an integral, resulting in

$$\sum_{n=0}^\infty f(n + \frac{1}{2}) = \int_0^\infty f(x) dx - \frac{1}{24} \left(\int_0^\infty f''(x) dx - \frac{1}{24} \sum_{n=0}^\infty f^{(iv)}(n + \frac{1}{2}) \right) + \dots,$$

and we obtain

EULER-MACLAURIN FORMULA
(leading order)

$$\sum_{n=0}^\infty f(n + \frac{1}{2}) = \int_0^\infty f(x) dx + \frac{1}{24} f'(0) - \frac{1}{24} f'(\infty) + \dots \quad (8.2)$$

These are actually the first terms of the *Euler MacLaurin formula*.

8.3 One-particle density of states

The one-particle density of states in D spatial dimensions is

$$\begin{aligned}
 \rho^{(D)}(\varepsilon) &= \sum_{\mathbf{k}} \delta\left(\varepsilon - \frac{\hbar^2 \mathbf{k}^2}{2m}\right) \\
 &= \frac{V^{(D)}}{(2\pi)^D} \int d^D \mathbf{k} \delta\left(\varepsilon - \left(\frac{\hbar \mathbf{k}}{\sqrt{2m}}\right)^2\right) \\
 &= \frac{V^{(D)}}{(2\pi)^D} \left(\frac{\sqrt{2m}}{\hbar}\right)^D \int d^D \mathbf{x} \delta(\varepsilon - \mathbf{x}^2) \\
 &= \frac{V^{(D)}(2m)^{D/2}}{(2\pi)^D \hbar^D} \Omega_D \int_0^\infty dx x^{D-1} \delta(\varepsilon - x^2) \\
 &= \frac{V^{(D)}(2m)^{D/2}}{(2\pi)^D \hbar^D} \Omega_D \theta(\varepsilon \geq 0) \int_0^\infty dx x^{D-1} \frac{\delta(x - \sqrt{\varepsilon})}{2x} \\
 &= \frac{V^{(D)}(2m)^{D/2}}{(2\pi)^D \hbar^D} \frac{\Omega_D}{2} \varepsilon^{\frac{D-2}{2}} \theta(\varepsilon \geq 0)
 \end{aligned}$$

In appendix C of the statistics I script we have derived the surface Ω_D of a D -dimensional hypersphere of unit radius

$$\Omega_D = \frac{2\pi^{D/2}}{\Gamma(D/2)} .$$

The D -dimensional dos of the free electron gas is therefore

DENSITY OF STATES
(*D*-dimensional free electron gas)

$$\rho^{(D)}(\varepsilon) = \frac{V^{(D)} m^{\frac{D}{2}}}{\hbar^D (2\pi)^{\frac{D}{2}} \Gamma(\frac{D}{2})} \varepsilon^{\frac{D-2}{2}} \theta(\varepsilon \geq 0) . \quad (8.3a)$$

$$\rho^{(1)}(\varepsilon) = \frac{L\sqrt{m}}{\hbar\sqrt{2\pi}} \frac{1}{\sqrt{\varepsilon}} \theta(\varepsilon \geq 0) . \quad (8.3b)$$

$$\rho^{(2)}(\varepsilon) = \frac{V^{(2)} m}{\hbar^2 2\pi} \theta(\varepsilon \geq 0) , \quad (8.3c)$$

$$\rho^{(3)}(\varepsilon) = \frac{Vm^{\frac{3}{2}}}{\hbar^3 \sqrt{2\pi^2}} \sqrt{\varepsilon} \theta(\varepsilon \geq 0) . \quad (8.3d)$$

8.4 Eigenvalues of the free electron gas in a homogeneous magnetic field

Here we determine the one-particle eigenvalues of the free electron gas in a homogeneous magnetic field. Since the electron do not interact with each other, it suffices to consider the hamiltonian of single electron, which reads

$$H = \frac{(\hat{\mathbf{p}} + e\hat{\mathbf{A}})^2}{2m} + \mu_B g_e \mathbf{B} \hat{\mathbf{S}} ,$$

where \mathbf{S} is the vector operator of the electronic spin. The direction of the magnetic field defines the z -direction. Since there is no spin-orbit coupling, the eigenvector is a tensor product of the orbital and spin degrees of freedom. For the latter the vector is the eigenvector of the operator S_z , i.e.

$$|\psi\rangle = |\Phi\rangle \otimes |\sigma\rangle$$

The eigenvalue problem turns into

$$H|\psi\rangle = |\sigma\rangle \otimes \left(\frac{(\hat{\mathbf{p}} + e\hat{\mathbf{A}})^2}{2m} + \underbrace{\frac{\mu_B \hbar g_e}{2}}_{=b} \sigma \right) |\Phi\rangle = \varepsilon |\sigma\rangle \otimes |\Phi\rangle$$

The orbital part of the eigenvalue problem reads

$$\frac{(\hat{\mathbf{p}} + e\hat{\mathbf{A}})^2}{2m} |\Phi\rangle = \varepsilon' |\Phi\rangle$$

8.4. EIGENVALUES OF THE FREE ELECTRON GAS IN A HOMOGENEOUS MAGNETIC FIELD

and the the eigenvalues of the entire hamitonian are

$$\varepsilon = \varepsilon' + b\sigma .$$

The vector potential for the homogeneous magnetic field in z -direction can be chosen (Landau gauge) as

$$\mathbf{A} = B(0, x, 0) .$$

We readily see that it gives the correct \mathbf{B} field

$$\begin{aligned} \mathbf{B} &= \nabla \times \mathbf{A} \\ &= \begin{pmatrix} \partial_y A_z - \partial_z A_y \\ \partial_z A_x - \partial_x A_z \\ \partial_x A_y - \partial_y A_x \end{pmatrix} \\ &= B \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} . \end{aligned}$$

Inserting \mathbf{A} into the orbital eigenvalue problem gives

$$\frac{\hat{p}_x^2 + (\hat{p}_y + eB\hat{x})^2 + \hat{p}_z^2}{2m} |\Phi\rangle = \varepsilon' |\Phi\rangle$$

The y and z coordinate only enters via the momenta, therefore, the eigenvector is a tensor product of the form

$$|\Phi\rangle = |\Phi_x\rangle \otimes |p_y\rangle \otimes |p_z\rangle ,$$

where $|k_x\rangle$ ($|k_x\rangle$) is an eigenvector of the momentum operator p_x (p_y) with the corresponding eigenvalue. Then

$$\begin{aligned} \frac{\hat{p}_x^2 + (\hat{p}_y + eB\hat{x})^2 + \hat{p}_z^2}{2m} |\Phi\rangle &= |p_y\rangle \otimes |p_z\rangle \otimes \frac{\hat{p}_x^2 + (p_y + eB\hat{x})^2 + p_z^2}{2m} |\Phi_x\rangle \\ &= |p_y\rangle \otimes |p_z\rangle \otimes \left(\varepsilon' |\Phi_x\rangle \right) \end{aligned}$$

The remaining 1D problem reads

$$\frac{\hat{p}_x^2 + (p_y + eB\hat{x})^2 + p_z^2}{2m} |\Phi_x\rangle = \varepsilon' |\Phi_x\rangle$$

The electron gas is confined to a box of size $L_x \times L_y \times L_y$. The momentum eigenvalues are therefore quantized as

$$p_y = \hbar \frac{2\pi}{L_y} n_y , \quad \text{with } n_y \in \mathbf{N} \quad (8.4)$$

$$p_z = \hbar \frac{2\pi}{L_z} n_z , \quad \text{with } n_z \in \mathbf{N} \quad (8.5)$$

$$(8.6)$$

The 1D hamiltonian can be rewritten in the form

$$\left(\frac{1}{2m} \hat{p}_x^2 + \frac{eB}{2m} \left(\hat{x} + \underbrace{\frac{p_y}{eB}}_{:= -x_0} \right)^2 + \frac{p_z^2}{2m} \right) |\Phi_x\rangle = \varepsilon' |\Phi_x\rangle$$

This is the hamiltonian of a harmonic oscillator shifted by x_0 . The prefactor of the x^2 term corresponds to $\omega_c/2$, hence $\omega_c = eB/m$. The eigenvalues of the harmonic oscillator yield

$$\varepsilon' = \frac{p_z^2}{2m} + \hbar\omega_c \left(n + \frac{1}{2} \right) .$$

These eigenvalues are independent of p_y and, therefore, degenerate. p_y defines the center x_0 of the harmonic oscillator, which has to be within $(0, L_x)$, resulting in the condition

$$\begin{aligned} 0 &\leq \frac{p_y}{eB} \leq L_x \\ 0 &\leq \frac{\hbar 2\pi}{L_y eB} n_y \leq L_x \\ 0 &\leq n_y \leq \frac{L_x L_y eB}{2\pi \hbar} . \end{aligned}$$

The number of allowed p_y values defines the degeneracy

$$N_{\text{deg}} = \left\lfloor \frac{L_x L_y eB}{2\pi \hbar} \right\rfloor + 1 .$$

This number will be much greater than 1 and we can, therefore, ignore the fact that it has to be an integer and we simply use

$$N_{\text{deg}} = \frac{L_x L_y eB}{2\pi \hbar} . \quad (8.7)$$

8.5 Langevin Diamagnetismus

Now we consider the entire free-electron gas model. The single electron energies are now

$$\begin{aligned} \varepsilon_{n,\sigma}(k_z) &= \varepsilon(k_z) + \hbar\omega_c \left(n + \frac{1}{2} \right) + \sigma b \\ \varepsilon(k_z) &= \frac{\hbar^2 k_z^2}{2m} \end{aligned}$$

with $b = \frac{\mu_B g_e}{2}$ and the cyclotron frequency $\omega_c = \frac{eB}{m}$, and $\mu_B = \frac{e\hbar}{2m}$. The degeneracy of these levels is

$$N_{\text{deg}} = \frac{L_x L_y eB}{2\pi \hbar} = BC_{\text{deg}} .$$

We use again the formula for the grand canonical partition function of non-interacting particles

$$\ln(Z) = \sum_{\nu} \ln(1 + e^{-\beta(\varepsilon_{\nu} - \mu)})$$

Inserting the one particle energies results in

$$\ln(Z) = BC_{deg} \sum_{\sigma} \sum_{n=0}^{\infty} \underbrace{\int d\varepsilon \rho^{(1d)}(\varepsilon) \ln \left(1 + e^{-\beta(\varepsilon + \hbar\omega_c(n + \frac{1}{2}) + b\sigma - \mu)} \right)}_{\substack{:= F(\mu - \hbar\omega_c(n + \frac{1}{2}) - b\sigma) \\ := f(n + \frac{1}{2})}}. \quad (8.8)$$

Now we invoke the leading Euler-Mac-Laurin formula in equation (8.2) [p. 186] to leading order and use $f'(\infty) = 0$.

$$\begin{aligned} \sum_{n=0}^{\infty} f(n + \tfrac{1}{2}) &= \int_0^{\infty} f(x) dx + \frac{1}{24} f'(0) + \dots \\ &= \int_0^{\infty} F(\mu - \hbar\omega_c x - b\sigma) dx + \frac{1}{24} \frac{\partial}{\partial x} F(\mu - \hbar\omega_c x - b\sigma) \Big|_{x=0} + \dots \\ &= \frac{1}{\hbar\omega_c} \int_0^{\infty} F(\mu - y - b\sigma) dy - \frac{\hbar\omega_c}{24} \frac{\partial}{\partial \mu} F(\mu - b\sigma) + \dots \end{aligned}$$

Next we expand this expression in terms of B , or rather b , up to second order. We also include already the sum over the electronic spin, which allows to omit term proportional to σ^m for odd m .

$$\begin{aligned} \sum_{\sigma} \sum_n f(n + \tfrac{1}{2}) &= \sum_{\sigma} \frac{1}{\hbar\omega_c} \left(\int_0^{\infty} F(\mu - y) dy - \cancel{b\sigma} \int_0^{\infty} \frac{\partial}{\partial \mu} F(\mu - y) dy + \right. \\ &\quad \left. + \frac{b^2}{2} \int_0^{\infty} \frac{\partial^2}{\partial \mu^2} F(\mu - y) dy - \frac{(\hbar\omega_c)^2}{24} \frac{\partial}{\partial \mu} F(\mu) + \mathcal{O}(B^4) \right) \\ &= \frac{2}{\hbar\omega_c} \left(\int_{-\infty}^{\mu} F(z) dz + \right. \\ &\quad \left. + \frac{b^2}{2} \int_0^{\infty} \frac{\partial^2}{\partial y^2} F(\mu - y) dy - \frac{(\hbar\omega_c)^2}{24} \frac{\partial}{\partial \mu} F(\mu) + \mathcal{O}(B^4) \right) \\ &= \frac{2}{\hbar\omega_c} \left(\int_{-\infty}^{\mu} F(z) dz + \right. \\ &\quad \left. + \frac{b^2}{2} \left(\frac{\partial}{\partial \mu} F(\mu - y) \right) \Big|_{y=0}^{y=\infty} - \frac{(\hbar\omega_c)^2}{24} \frac{\partial}{\partial \mu} F(\mu) + \mathcal{O}(B^4) \right) \\ &= \frac{2}{\hbar\omega_c} \left(\int_{-\infty}^{\mu} F(z) dz + \frac{1}{2} \left(b^2 - \frac{(\hbar\omega_c)^2}{12} \right) \frac{\partial}{\partial \mu} F(\mu) + \mathcal{O}(B^4) \right). \end{aligned}$$

Inserting the definition of ω_c and b yields

$$\begin{aligned} b^2 - \frac{(\hbar\omega_c)^2}{12} &= B^2 \left(\mu_B^2 \left(\frac{g_e}{2} \right)^2 - \frac{1}{12} \left(\frac{\hbar e}{m} \right)^2 \right) \\ &= B^2 \mu_B^2 \left(\left(\frac{g_e}{2} \right)^2 - \frac{4}{12} \right) \end{aligned}$$

The grand potential up to order B^2 reads

$$\begin{aligned} \Omega &= -k_B T \ln(Z) \\ &= - \underbrace{\frac{2k_B T C_{deg} B}{\hbar\omega_c}}_{=D} \left(\int_0^\infty F(\mu - y) dy + \frac{\mu_B^2 B^2}{2} \left(\left(\frac{g_e}{2} \right)^2 - \frac{4}{12} \right) \frac{\partial}{\partial \mu} F(\mu) \right) \\ &= D \int_0^\infty F(\mu - y) dy + \frac{1}{2} \left(\left(\frac{g_e}{2} \right)^2 - \frac{4}{12} \right) D \frac{\partial}{\partial \mu} F(\mu) . \end{aligned}$$

For $B = 0$ we obtain

$$\Omega(T, \mu, B = 0) = D \int_0^\infty F(\mu - y) dy$$

We can exploit

$$\begin{aligned} \frac{\partial}{\partial \mu} \int_{-\infty}^\mu F(z) dz &= F(\mu) \\ \Rightarrow \quad \frac{\partial}{\partial \mu} F(\mu) &= \frac{\partial^2}{\partial \mu^2} \int_{-\infty}^\mu F(z) dz \end{aligned}$$

to rewrite the grand potential as

$$\Omega(T, \mu, B) = \Omega(T, \mu, B = 0) + \frac{\mu_B^2 B^2}{2} \left(\left(\frac{g_e}{2} \right)^2 - \frac{1}{3} \right) \frac{\partial^2}{\partial \mu^2} \Omega(T, \mu, B = 0) .$$

The susceptibility is defined as

$$\chi = - \frac{\partial \Omega}{\partial B^2} \Big|_{\mu, T} = - \mu_B^2 \left(\left(\frac{g_e}{2} \right)^2 - \frac{1}{3} \right) \frac{\partial^2}{\partial \mu^2} \Omega(T, \mu, B = 0) ,$$

Finally, we exploit the equation $\frac{\partial \Omega}{\partial \mu} \Big|_{T, B} = N(T, \mu, B)$ resulting in

$$\chi = - \frac{\partial \Omega}{\partial B^2} \Big|_{\mu, T} = \left(1 - \frac{1}{3} \left(\frac{2}{g_e} \right)^2 \right) \left(\mu_B^2 \left(\frac{g_e}{2} \right)^2 \frac{\partial}{\partial \mu} N(T, \mu, B = 0) \right) ,$$

According to equation (6.38) [p. 157] the last bracket is equal to the Pauli-spin susceptibility, i.e.

$$\chi = \chi_P - \frac{1}{3} \left(\frac{2}{g_e} \right)^2 \chi_P$$

The additional term is called *Landau Diamagnetism* and for $g_e \approx 2$ is is

$$\chi_L = -\frac{1}{3} \chi_P$$

The total susceptibility is still positive

$$\chi \approx \frac{2}{3} \chi_P .$$

8.6 Bogoliubov inequality

Here we will prove the Bogoliubov inequality. To this end we will exploit the Schwarz inequality

$$|(A|B)|^2 \leq (A|A)(B|B) , \quad (8.9)$$

where $(X|Y)$ are scalar products between any vectors A and B . To be able to use this relation, we have to introduce a suitable scalar product, that involves the operators A and B

$$(A|B) := \sum_{n,m}^{E_m \neq E_n} \langle m|A^\dagger|n\rangle \langle n|B|m\rangle \frac{\rho_m - \rho_n}{E_n - E_m}$$

with

$$\rho_m = \frac{e^{-\beta E_m}}{\text{tr} \{e^{-\beta H}\}} .$$

This product fulfils the four defining properties of a scalar product

- $(A|B) = (B|A)^*$.

This is obviously the case

$$\begin{aligned} (B|A)^* &= \sum_{n,m}^{E_m \neq E_n} (\langle m|B^\dagger|n\rangle \langle n|A|m\rangle)^* \frac{\rho_m - \rho_n}{E_n - E_m} \\ &= \sum_{n,m}^{E_m \neq E_n} \langle m|A^\dagger|n\rangle \langle n|B|m\rangle \frac{\rho_m - \rho_n}{E_n - E_m} , \\ &= (A|B) . \quad \checkmark \end{aligned}$$

- Linearity $(A|\alpha B_1 + \beta B_2) = \alpha(A|B_1) + \beta(A|B_2)$, which follows from the linearity of the matrix elements $\langle n|B|m\rangle$.
- $(A|A) \geq 0$, since

$$(A|A) = \sum_{n,m}^{E_m \neq E_n} \underbrace{|\langle n|A^\dagger|m\rangle|^2}_{\geq 0} \underbrace{\frac{\rho_m - \rho_n}{E_n - E_m}}_{\geq 0}.$$

- From $A = 0$ follows clearly $(A|A) = 0$, but not conversely

So we can conclude that $(A|B)$ is a semi-definite scalar product, for which the Schwarz inequality applies. In addition, the product has the special feature

$$(H|A) = 0, \quad \forall \text{ operators } A. \quad (8.10)$$

This is easily seen, since $\langle m|H^\dagger|n\rangle = E_n\delta_{mn}$; but $m = n$ is excluded from the sum.

Next we exploit it for the prove of the Bogoliubov inequality. To this end, we first use $B = [C^\dagger, H]$ in the Schwarz relation. For the lhs we need $(A|B)$

$$\begin{aligned} (A|B) &= (A|[C^\dagger, H]) \\ &= \sum_{mn}^{E_m \neq E_n} \langle m|A^\dagger|n\rangle \langle n|[C^\dagger, H]|m\rangle \frac{\rho_m - \rho_n}{E_n - E_m} \\ &= \sum_{mn}^{E_m \neq E_n} \langle m|A^\dagger|n\rangle \langle n|C^\dagger|m\rangle (E_m - E_n) \frac{\rho_n - \rho_m}{E_m - E_n} \\ &= \sum_{mn}^{E_m \neq E_n} \langle m|A^\dagger|n\rangle \langle n|C^\dagger|m\rangle (\rho_n - \rho_m). \end{aligned}$$

Now we can omit the restriction in the sum, since $(\rho_n - \rho_m)$ is zero for $n = m$, anyways. Then

$$(A|B) = \sum_{mn} \rho_n \langle n|C^\dagger|m\rangle \langle m|A^\dagger|n\rangle - \sum_{mn} \rho_m \langle m|A^\dagger|n\rangle \langle n|C^\dagger|m\rangle.$$

Renaming $n \leftrightarrow m$ in the last term eventually leads to

$$(A|B) = \left\langle [C^\dagger, A^\dagger]_- \right\rangle \quad (8.11)$$

If we also choose $A = B = [C^\dagger, H]_-$ in equation (8.11), we obtain

$$(B|B) = \left\langle [C^\dagger, [H, C]_-]_- \right\rangle = \left\langle [[C, H], C^\dagger]_- \right\rangle \geq 0. \quad (8.12)$$

For the next steps we use ($\rho_m = e^{-\beta E_m}/Z$)

$$\rho_m > \rho_n \quad \text{if} \quad E_n > E_m .$$

Hence, for any $E_n \neq E_m$

$$0 < \frac{\rho_m - \rho_n}{E_n - E_m} = \frac{\rho_m + \rho_n}{E_n - E_m} \cdot \frac{\rho_m - \rho_n}{\rho_m + \rho_n} . \quad (8.13)$$

The second factor can be modified

$$\begin{aligned} \frac{\rho_m - \rho_n}{\rho_m + \rho_n} &= \frac{e^{-\beta E_m} - e^{-\beta E_n}}{e^{-\beta E_m} + e^{-\beta E_n}} \\ &= \frac{e^{-\frac{\beta}{2} E_m} e^{-\frac{\beta}{2} E_n} \left(e^{-\frac{\beta}{2} (E_m - E_n)} - e^{-\frac{\beta}{2} (E_n - E_m)} \right)}{e^{-\frac{\beta}{2} E_m} e^{-\frac{\beta}{2} E_n} \left(e^{-\frac{\beta}{2} (E_m - E_n)} + e^{-\frac{\beta}{2} (E_n - E_m)} \right)} \\ &= \tanh \left(\frac{\beta}{2} (E_n - E_m) \right) \end{aligned}$$

Then equation (8.13) yields

$$0 < \frac{\rho_m - \rho_n}{E_n - E_m} = \frac{\beta}{2} (\rho_m + \rho_n) \frac{\tanh \left(\frac{\beta}{2} (E_n - E_m) \right)}{\frac{\beta}{2} (E_n - E_m)} .$$

Since $\tanh(x)/x < 1$, we find

$$0 < \frac{\rho_m - \rho_n}{E_n - E_m} < \frac{\beta}{2} (\rho_m + \rho_n) .$$

From this relation we obtain

$$(A|A) = \sum_{mn}^{E_m \neq E_n} \langle n|A^\dagger|m\rangle \langle m|A|n\rangle \frac{\rho_m - \rho_n}{E_n - E_m} < \frac{\beta}{2} \sum_{mn}^{E_m \neq E_n} \langle n|A^\dagger|m\rangle \langle m|A|n\rangle (\rho_m + \rho_n) .$$

The omitted terms for $E_n = E_m$ are positive, so including them does not violate the inequality

$$(A|A) < \frac{\beta}{2} \sum_{mn} \langle n|A^\dagger|m\rangle \langle m|A|n\rangle (\rho_m + \rho_n) = \frac{\beta}{2} \langle [A^\dagger, A]_+ \rangle \quad (8.14)$$

Now we return to the Schwarz inequality in equation (8.9) [\[p. 193\]](#)

$$|(A|B)|^2 \leq (A|A)(B|B) , \quad (8.15)$$

and insert piece by piece the relations we just derived for the various terms. Beginning with equation (8.11) [\[previous page\]](#) and equation (8.12) [\[previous page\]](#) we get

$$|\langle [C, A] \rangle|^2 \leq (A|A) \left\langle [[C, H], C^\dagger]_- \right\rangle ,$$

Along with equation (8.14) we finally obtain

$$|\langle [C, A] \rangle|^2 \leq \frac{\beta}{2} \langle [A^\dagger, A]_+ \rangle \left\langle [[C, H], C^\dagger]_- \right\rangle , \quad (8.16)$$

which proves the Bogoliubov inequality.

8.7 Proof used for the Bogoliubov inequality

Here we prove the relation

$$\left\langle [[C, H]_-, C^\dagger]_- \right\rangle \leq 4\hbar^2 N \left(|b\mathcal{S}_{\mathbf{Q}}(T, b)| + \mathbf{k}^2 X \right) . \quad (8.17)$$

We recall that

$$C = S_{\mathbf{k}}^+ = \sum_l e^{i\mathbf{k}\mathbf{R}_l} S_l^+ .$$

Hence We begin with $[S_{\mathbf{k}}^+, H]_-$

$$\begin{aligned} [C, H_H]_- &= [S_{\mathbf{k}}^+, H_H]_- \\ &= - \sum_l e^{i\mathbf{R}_l \mathbf{k}} \sum_{jj'} J_{jj'} \left([S_l^+, S_j^+ S_{j'}^-] + [S_l^+, S_j^z S_{j'}^z] \right) \\ &= - \sum_l e^{i\mathbf{R}_l \mathbf{k}} \sum_{jj'} J_{jj'} \left(S_j^+ [S_l^+, S_{j'}^-] + S_j^z [S_l^+, S_{j'}^z] + [S_l^+, S_j^z] S_{j'}^z \right) \\ &= -\hbar \sum_l e^{i\mathbf{R}_l \mathbf{k}} \sum_{jj'} J_{jj'} \left(2S_j^+ \delta_{lj'} S_l^z - S_j^z \delta_{lj'} S_l^+ - \delta_{lj} S_l^+ S_{j'}^z \right) \\ &= -\hbar \sum_l e^{i\mathbf{R}_l \mathbf{k}} \sum_j J_{jl} \left(2S_j^+ S_l^z - S_j^z S_l^+ - S_l^+ S_j^z \right) \\ &= -2\hbar \sum_l e^{i\mathbf{R}_l \mathbf{k}} \sum_j J_{jl} \left(S_j^+ S_l^z - S_l^+ S_j^z \right) . \end{aligned}$$

We have used the symmetry $J_{jj'} = J_{j'l}$ and $S_j^z S_l^+ = S_l^+ S_j^z + [S_j^z, S_l^+]$. The commutator is proportional to δ_{jl} and hence to J_{jj} , which is zero. Meanwhile we have

$$[C, H_H]_- = -2\hbar \sum_{lj} (e^{i\mathbf{R}_l \mathbf{k}} - e^{i\mathbf{R}_j \mathbf{k}}) J_{jl} S_j^+ S_l^z.$$

We continue with the second commutator

$$[[C, H_H]_-, C^\dagger]_- = -2\hbar \sum_{lj} (e^{i\mathbf{R}_l \mathbf{k}} - e^{i\mathbf{R}_j \mathbf{k}}) J_{jl} \sum_{l'} e^{-i\mathbf{k} \mathbf{R}_{l'}} [S_j^+ S_l^z, S_{l'}^-].$$

With

$$\begin{aligned} [S_j^+ S_l^z, S_{l'}^-] &= S_j^+ [S_l^z, S_{l'}^-] + [S_j^+, S_{l'}^-] S_l^z \\ &= -\delta_{ll'} \hbar S_j^+ S_l^- + 2\hbar \delta_{l'l} S_j^z S_l^z \end{aligned}$$

we obtain

$$\begin{aligned} [[C, H_H]_-, C^\dagger]_- &= -2\hbar^2 \sum_{lj} (e^{i\mathbf{R}_l \mathbf{k}} - e^{i\mathbf{R}_j \mathbf{k}}) J_{jl} \left(-e^{-i\mathbf{k} \mathbf{R}_l} S_j^+ S_l^- + 2e^{-i\mathbf{k} \mathbf{R}_j} S_j^z S_l^z \right) \\ &= 2\hbar^2 \sum_{lj} J_{jl} \left((1 - e^{i(\mathbf{R}_j - \mathbf{R}_l) \mathbf{k}}) S_j^+ S_l^- - 2(e^{-i(\mathbf{R}_j - \mathbf{R}_l) \mathbf{k}} - 1) S_j^z S_l^z \right) \\ &= 2\hbar^2 \sum_{lj} J_{jl} \left(1 - e^{i(\mathbf{R}_j - \mathbf{R}_l) \mathbf{k}} \right) \left(S_j^+ S_l^- + 2S_j^z S_l^z \right). \end{aligned}$$

In the last step we have substituted $j \leftrightarrow l$ and used the symmetry of J_{jl} . Finally, we repeat the calculation for the field term

$$\begin{aligned} [C, H_b]_- &= [S_{\mathbf{k}}^+, H_b]_- = b \sum_{ll'} e^{i\mathbf{R}_l \mathbf{k}} e^{i\mathbf{R}_{l'} \mathbf{Q}} \underbrace{[S_l^+, S_{l'}^z]}_{=-\delta_{ll'} \hbar S_l^+} \\ &= b\hbar \sum_l e^{i\mathbf{R}_l (\mathbf{k} + \mathbf{Q})} S_l^+. \end{aligned}$$

Then

$$\begin{aligned} [[C, H_b]_-, C^\dagger] &= b\hbar \sum_l e^{i\mathbf{R}_l (\mathbf{k} + \mathbf{Q})} \sum_{l'} e^{-i\mathbf{k} \mathbf{R}_{l'}} \underbrace{[S_l^+, S_{l'}^-]}_{=\delta_{ll'} 2\hbar S_l^z} \\ &= 2b\hbar^2 \sum_l e^{i\mathbf{R}_l \mathbf{Q}} S_l^z \\ &= 2b\hbar^2 S_{\mathbf{Q}}^z \\ &= 2bN\hbar^2 \mathcal{S}_{\mathbf{Q}}(T, b). \end{aligned}$$

Hence for $C = C_{\mathbf{k}}$ we have

$$\begin{aligned}
\left\langle [[C_{\mathbf{k}}, H]_-, C_{\mathbf{k}}^\dagger] \right\rangle &= 2bN\hbar^2 \mathcal{S}_Q(T, b) \\
&+ 2\hbar^2 \sum_{lj} J_{jl} \left(1 - e^{i(\mathbf{R}_j - \mathbf{R}_l)\mathbf{k}} \right) \left(\underbrace{\langle S_j^+ S_l^- \rangle + \langle S_j^z S_l^z \rangle}_{=\langle \mathbf{S}_j \cdot \mathbf{S}_l \rangle} + \langle S_j^z S_l^z \rangle \right) \\
&= 2bN\hbar^2 \mathcal{S}_Q(T, b) \\
&+ 2\hbar^2 \sum_{lj} J_{jl} \left(1 - e^{i(\mathbf{R}_j - \mathbf{R}_l)\mathbf{k}} \right) \left(\langle \mathbf{S}_j \cdot \mathbf{S}_l \rangle + \langle S_j^z S_l^z \rangle \right).
\end{aligned}$$

From equation (8.12) [p. 194] we know that $[[C, H_b]_-, C^\dagger]$ originates from the scalar product $(B|B)$. It is therefore a real and non-negative function for all \mathbf{k} . Then

$$\begin{aligned}
\left\langle [[C_{\mathbf{k}}, H]_-, C_{\mathbf{k}}^\dagger] \right\rangle &\leq \left\langle [[C_{\mathbf{k}}, H]_-, C_{\mathbf{k}}^\dagger] \right\rangle + \left\langle [[C_{-\mathbf{k}}, H]_-, C_{-\mathbf{k}}^\dagger] \right\rangle \\
\left\langle [[C_{\mathbf{k}}, H]_-, C_{\mathbf{k}}^\dagger] \right\rangle &\leq 4b\hbar^2 N \mathcal{S}_Q(T, b) \\
&+ 4\hbar^2 \sum_{lj} J_{jl} \left(1 - \cos(\mathbf{R}_j - \mathbf{R}_l)\mathbf{k} \right) \left(\langle \mathbf{S}_j \cdot \mathbf{S}_l \rangle + \langle S_j^z S_l^z \rangle \right) \\
&\leq 4N\hbar^2 |b\mathcal{S}_Q(T, b)| \\
&+ 4\hbar^2 \sum_{lj} \underbrace{|J_{jl}| \left(1 - \cos(\mathbf{R}_j - \mathbf{R}_l)\mathbf{k} \right)}_{\geq 0} \left(|\langle \mathbf{S}_j \cdot \mathbf{S}_l \rangle| + |\langle S_j^z S_l^z \rangle| \right).
\end{aligned}$$

Finally, we can use the Schwarz inequality for the scalar products $\langle \mathbf{S}_j \cdot \mathbf{S}_l \rangle$

$$\begin{aligned}
|\langle \mathbf{S}_j \cdot \mathbf{S}_l \rangle|^2 &\leq \langle \mathbf{S}_j^2 \rangle \langle \mathbf{S}_l^2 \rangle = \left(\hbar^2 S(S+1) \right)^2 \\
|\langle \mathbf{S}_j \cdot \mathbf{S}_l \rangle| &\leq \hbar^2 S(S+1).
\end{aligned}$$

Moreover, $|\langle S_j^z S_l^z \rangle| \leq |\langle S_j S_l \rangle| \leq \hbar^2 S(S+1)$. In total we have

$$\left\langle [[C, H]_-, C^\dagger] \right\rangle \leq 4N\hbar^2 \left(|b\mathcal{S}_Q(T, b)| + 2S(S+1)\hbar^2 \frac{1}{N} \sum_{jl} |J_{jl}| \left(1 - \cos(\mathbf{R}_j - \mathbf{R}_l)\mathbf{k} \right) \right)$$

Moreover we use

$$1 - \cos(x) \leq \frac{x^2}{2},$$

and obtain

$$\langle [[C, H]_-, C^\dagger] \rangle \leq 4N\hbar^2 \left(|b\mathcal{S}_Q(T, b)| + \underbrace{\mathbf{k}^2 \frac{S(S+1)\hbar^2}{N} \sum_{jl} |J_{jl}| |\mathbf{R}_j - \mathbf{R}_l|^2}_{=X \text{ with } 0 \leq X < \infty} \right)$$

Which proves equation (8.17) [\[p. 196\]](#).

Chapter 9

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