1 Canonical treatment of paramagnetism *(6 points)*

As a classical model for paramagnetism one can consider a system of N particles with the Hamiltonian

$$\mathcal{H} = -hM \quad \text{with} \quad M = \mu \cdot \sum_{i=1}^{N} \cos\theta_i \tag{1}$$

where h is an external homogeneous magnetic field, μ the magnetic moment of a single particle and θ_i the angle between the magnetic field h and the magnetic moment μ of particle i.

1. Use the canonical distribution to calculate the average magnetization, $\langle M \rangle$, as a function of h and temperature T. *(3 points)*

Partition function:

$$Z = Z_0 \cdot \left(\int \mathrm{d}^N\Omega \; e^{h\beta\mu \sum_i^N \cos\theta_i} \right) \tag{2}$$

$$= Z_0 \cdot \left(\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \cdot \sin\theta \cdot e^{h\beta\mu\cos\theta} \right)^N \tag{3}$$

$$= Z_0 \cdot \left(\frac{4\pi \cdot \sinh(\beta\mu h)}{\beta\mu h} \right)^N \tag{4}$$

Here, Z_0 is the part of the partition function that does not include the integration over orientations.

Free energy:

$$F = -k_B T \ln(Z) \tag{5}$$

$$= -k_B T \cdot \Big(\ln(Z_0) + N\ln(4\pi) \Big) - N k_B T \ln\left(\frac{\sinh(\beta\mu h)}{\beta\mu h} \right) \tag{6}$$

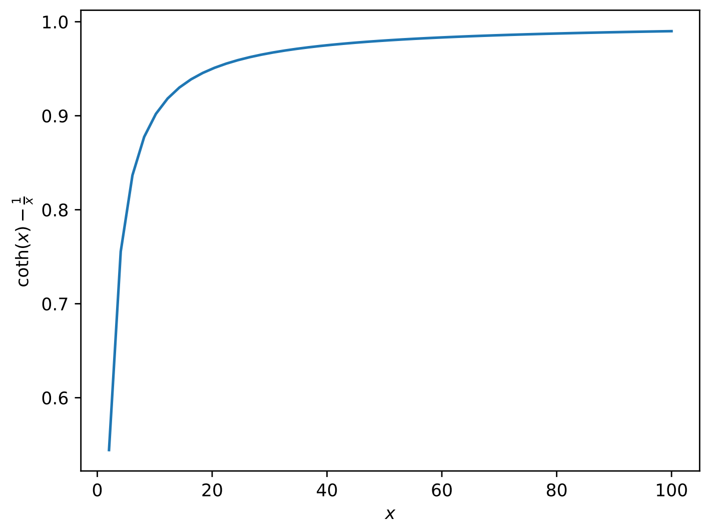
Magnetization:

$$M = -\frac{\partial F}{\partial h}\bigg|_{T,V,N} = N\mu \cdot \left(\coth(x) - \frac{1}{x} \right) \tag{7}$$

with $x := \beta\mu h$.

2. The ratio of which quantities determines the average magnetization? Sketch the functional dependence of the average magnetization on this ratio. ***(1 point)***

The average magnetization is determined by the ratio $\beta\mu h = \mu h/k_B T$.



3. Discuss the two limiting cases: high temperature/weak field vs. low temperature/strong field. ***(2 points)***

For $T \to 0$, i.e. $x \to \infty$:

$$\coth(x) = \frac{e^{2x}+1}{e^{2x}-1} \approx \frac{e^{2x}}{e^{2x}} = 1 \qquad \text{and} \qquad 1/x \to 0 \tag{8}$$

$$\Rightarrow M \approx N\mu \tag{9}$$

As expected, all spins are aligned to the external magnetic field.

For $T \to \infty$, i.e. $x \to 0$:

$$\coth x = \frac{e^{2x}+1}{e^{2x}-1} \to \frac{1}{x} \qquad \text{(Laurent power series)} \tag{10}$$

which actually cancels the divergence $-1/x$ and thus

$$\Rightarrow M \approx \frac{1}{2}N\beta\mu^2 h \to 0 \tag{11}$$

For high temperatures, the mean magnetization is zero, due to the non-uniform distribution of θ_i.

2 One-dimensional lattice gas *(6 points)*

Consider a one-dimensional lattice model for a non-ideal gas with N lattice sites and periodic boundary conditions. Each lattice site i is either empty (occupancy $n_i = 0$) or occupied by at most one atom (occupancy $n_i = 1$). There is an attractive energy J between atoms occupying neighbouring sites. The chemical potential of the atoms is μ. The Hamiltonian of this lattice gas is

$$H = -J \cdot \sum_{\langle ij \rangle} n_i n_j - \mu \cdot \sum_i n_i \,, \tag{12}$$

where $\sum_{\langle ij \rangle}$ is the sum over all pairs of neighbouring sites.

1. Express the partition sum of the one-dimensional lattice gas in terms of the transfer matrix T. Calculate the transfer matrix T and its eigenvalues. ***(2 points)***

The partition sum is given by

$$Z_N = \sum_{\{n_i\}} e^{-\beta H} = \sum_{n_1=0,1} \dots \sum_{n_N=0,1} e^{-\beta H} \,. \tag{13}$$

Let us rewrite the Hamiltonian in the following manner:

$$\begin{aligned} H &= -J \sum_{\langle ij \rangle} n_i n_j - \mu \sum_{i=1}^{N} n_i \\ &= -J \sum_{i=1}^{N} n_i n_{i+1} - \frac{1}{2}\mu \sum_{i=1}^{N} (n_i + n_{i+1}) \,. \end{aligned} \tag{14}$$

This is equivalent since we have periodic boundary conditions ($n_{N+1} = n_1$) and the lattice is one-dimensional. Now, we can define

$$-\beta H = K \sum_{i=1}^{N} n_i n_{i+1} + \frac{1}{2} L \sum_{i=1}^{N} (n_i + n_{i+1}) \,, \tag{15}$$

where $K = \beta J$ and $L = \beta \mu$. This allows us to write the argument of the partition sum as

$$e^{-\beta H} = T_{1,2} \cdot T_{2,3} \cdot \dots \cdot T_{N,1} \,, \tag{16}$$

where

$$T_{i,i+1} = e^{K n_i n_{i+1} + \frac{1}{2} L (n_i + n_{i+1})} \tag{17}$$

is the transfer matrix from lattice site i to site $i+1$. From the fact that there are two possible values for n_i and n_{i+1} (unoccupied or occupied) which are independent of the index i, one can conclude that the 2×2 transfer matrix is independent of the index i. Thus, one can write

$$T = \begin{bmatrix} 1 & e^{\frac{1}{2}L} \\ e^{\frac{1}{2}L} & e^{K+L} \end{bmatrix} \,, \tag{18}$$

where T_{00} corresponds to $n_i = n_{i+1} = 0$, T_{01} corresponds to $n_i = 0$ and $n_{i+1} = 1$, T_{10} corresponds to $n_i = 1$ and $n_{i+1} = 0$ and T_{11} corresponds to $n_i = n_{i+1} = 1$. Since the transfer matrix is independent of the index i, on can simplify the partition sum further by defining

$$|n_i = 0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} , \tag{19}$$

$$|n_i = 1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} . \tag{20}$$

With this definition it follows that $\sum_{n_i=0,1} |n_i\rangle\langle n_i| = 1$ and

$$\begin{aligned} Z_N &= \sum_{n_1=0,1} ... \sum_{n_N=0,1} T_{1,2} \cdot T_{2,3} \cdot ... \cdot T_{N,1} && (21) \\ &= \sum_{n_1=0,1} ... \sum_{n_N=0,1} \langle n_1|T|n_2\rangle\langle n_2|T|n_3\rangle ... \langle n_N|T|n_1\rangle && (22) \\ &= \sum_{n_1=0,1} \langle n_1|T^N|n_1\rangle && (23) \\ &= \lambda_1^N(K, L) + \lambda_2^N(K, L) , && (24) \end{aligned}$$

where λ_1 and λ_2 are the eigenvalues of T which are given by

$$\lambda_{1/2}(K, L) = \frac{1 + e^{K+L} \pm \sqrt{(1 + e^{K+L})^2 - 4e^L(e^K - 1)}}{2} . \tag{25}$$

2. Find a transformation of the occupancies n_i to map the lattice gas model to the Ising model with spins s_i. *(2 points)*

A map from the lattice gas model,

$$Z_L(K, L) = \sum_{\{n_i\}} e^{K \sum_i n_i n_{i+1} + L \sum_i n_i} , \tag{26}$$

with occupancies $n_i = 0, 1$ to the Ising model,

$$Z_I(K', L') = \sum_{\{s_i\}} e^{K' \sum_i s_i s_{i+1} + L' \sum_i s_i} , \tag{27}$$

with spins $s_i = \pm 1$ can be given by

$$n_i = \frac{s_i + 1}{2} . \tag{28}$$

Inserting Eq. (28) into Eq. (26) yields

$$Z_L(K, L) = e^{\frac{N}{2}(\frac{K}{2}+L)} \cdot Z_I\left(K'(K, L), L'(K, L)\right) , \tag{29}$$

with $K'(K, L) = K/4$ and $L'(K, L) = (K + L)/2$. Thus, the lattice gas model and the Ising model are in fact equivalent since the partition sum changes only by a constant prefactor. Expressing the eigenvalues of the lattice model $\lambda_{1/2}(K, L)$ with the new variables K' and L',

$$\lambda_{1/2}\left(K', L'\right) = e^{L'} \left(\cosh(L') \pm \sqrt{\cosh^2(L') - 2e^{-2K'} \sinh(2K')}\right) , \tag{30}$$

and calculating the partition sum of the Ising model,

$$\begin{aligned} Z_I\left(K', L'\right) &= e^{-N(L'-K')}\, Z_L(K', L') = e^{-N(L'-K')} \left(\lambda_1^N\left(K', L'\right) + \lambda_2^N\left(K', L'\right)\right) \\ &= \tilde{\lambda}_1^N\left(K', L'\right) + \tilde{\lambda}_2^N\left(K', L'\right) , \end{aligned} \tag{31}$$

gives in fact the correct eigenvalues of the Ising model:

$$\tilde{\lambda}_{1/2}\left(K', L'\right) = e^{K'} \left(\cosh(L') \pm \sqrt{\cosh^2(L') - 2e^{-2K'} \sinh(2K')}\right) . \tag{32}$$

3. Derive an expression for the average $\langle n_i \rangle$ in the limit of $N \to \infty$ in terms of the eigenvalues of the transfer matrix. ***(2 points)***

Since $\lambda_1 > \lambda_2$ the partition sum can be simplified for $N \to \infty$:

$$Z = \lambda_1^N + \lambda_2^N = \lambda_1^N \left[1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N\right] \longrightarrow \lambda_1^N \,. \tag{33}$$

We see that only λ_1 matters in the limit $N \to \infty$. Thus, we will neglect $(\lambda_2/\lambda_1)^N$ in the following. An expression for $\langle n_i \rangle$ can be given as:

$$\begin{aligned}
\langle n_i \rangle &= \frac{1}{Z} \sum_{n_1=0,1} \dots \sum_{n_N=0,1} n_i \, e^{-\beta H} \\
&= \frac{1}{Z} \sum_{n_1=0,1} \dots \sum_{n_N=0,1} n_i \, T_{1,2} \cdot T_{2,3} \cdot \dots \cdot T_{N,1} \\
&= \frac{1}{Z} \sum_{n_1=0,1} \dots \sum_{n_N=0,1} \langle n_1|T|n_2\rangle \dots n_i \, \langle n_i|T|n_{i+1}\rangle \dots \langle n_N|T|n_1\rangle \\
&= \frac{1}{Z} \sum_{n_1=0,1} \langle n_1|T^{i-1} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} T^{N-(i-1)}|n_1\rangle \\
&= \frac{1}{Z} \operatorname{tr}\left(T^N \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}\right) \\
&= \frac{1}{Z} \operatorname{tr}\left(\begin{bmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{bmatrix} U^{-1} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} U\right) ,
\end{aligned} \tag{34}$$

where U is the matrix whose ith column is the eigenvector v_i of T:

$$v_1 = \begin{bmatrix} -e^{-\frac{L}{2}} \left(e^{K+L} - \lambda_1\right) \\ 1 \end{bmatrix} , \quad v_2 = \begin{bmatrix} -e^{-\frac{L}{2}} \left(e^{K+L} - \lambda_2\right) \\ 1 \end{bmatrix} . \tag{35}$$

Thus, we have in the limit $N \to \infty$:

$$\langle n_i \rangle = \frac{e^{K+L} - \lambda_2}{\lambda_1 - \lambda_2} = \frac{\lambda_1 - 1}{\lambda_1 - \lambda_2} \,. \tag{36}$$

Addition: It's easier if you use a small trick here.
The average $\langle n_i \rangle$ can be calculated through the sum of all occupation numbers:

$$\langle n_i \rangle = \frac{1}{N} \left\langle \sum_{i=1}^{N} n_i \right\rangle = \frac{1}{N} \, \partial_L \ln Z = \partial_L \ln \lambda_1 = \frac{\lambda_1 - 1}{\lambda_1 - \lambda_2} \,. \tag{37}$$

Both methods yield the same result but you don't need to compute the eigenvectors with the latter.

3 Renormalization of the Ising chain *(3 points)*

In the lecture we have derived the following RG flow equation for the coupling constant K of the Ising chain without magnetic field: the new value K' is given by

$$K'(K) = \frac{1}{2} \ln \cosh(2K). \tag{38}$$

In addition we have derived the absolute increase in free energy per spin arising in each iteration:

$$g(K) = \frac{1}{2} \ln 2 + \frac{1}{4} \ln \cosh(2K) \tag{39}$$

1. Write a short computer program (e.g. in Mathematica or Python) that defines the flow equation $K'(K)$ and the free energy increase $g(K)$ as functions. Start with a coupling constant $K_0 = 1$ and iterate through K_1, K_2, K_3 up to K_4. Also calculated the corresponding values $g_0 = g(K_0)$ to $g_4 = g(K_4)$. What are the limits for these two series? ***(1.5 points)***

Python functions:

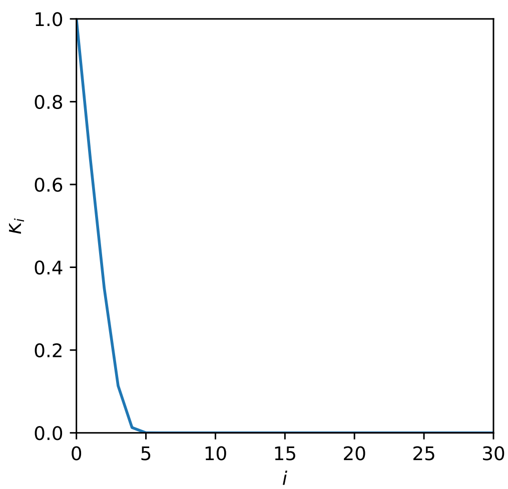
```python
def K_new(K):
    return log(cosh(2*K)) / 2


def g(K):
    return log(2) / 2 + log(cosh(2*K)) / 4
```

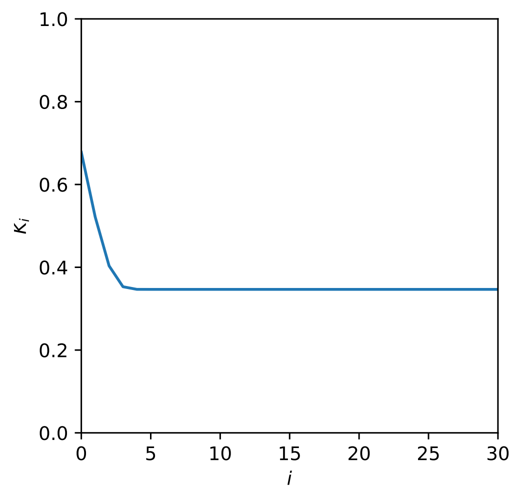
Iteration to $i = 4$ yields

	i=0	i=1	i=2	i=3	i=4
K_i	1	0.66	0.35	0.11	0.01
g_i	0.68	0.52	0.4	0.35	0.35

The K_i-series converges to zero for large i, while the g_i-series converges to $\frac{1}{2} \ln 2 \approx 0.35$.



(a) coupling constant K



(b) free energy increase g

2. Use these results to estimate the dimensionless free energy per spin $f = -\beta F/N$ in fourth order (simply cut the appropriate sum after the term with g_4; you can also include the next order term, but now by simply using the first term in $g(K)$). Compare to the known exact result for the Ising chain. How good is the numerical agreement? *(1.5 points)*

Our result by summing the series for g:

$$f = \sum_{i=0}^{4} \frac{g_i}{2^i} \approx 1.106\,. \tag{40}$$

Compare to exact result $f = \ln\left(2\cosh(K)\right) = 1.127$ for $K = 1$.