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13 Task Theoretical Physics VI - Statistics

13.1 (Exact solution of the Ising model in $d = 1$)

a)

We first want to show, that the partition function can be written as:

$$\begin{aligned} Z_N(T, B_0) &= \sum_{S_1, S_2, \ldots, S_N} e^{\beta \sum_i (g\mu_B B_0 S_i + J S_i S_{i+1})} \\ &= \sum_{S_1, S_2, \ldots, S_N} \tau(S_1, S_2)\, \tau(S_2, S_3) \ldots \tau(S_N, S_1) \end{aligned}$$

the Hamiltonian is given with

$$\hat{H} = -J \sum_{i=1}^{N-1} \hat{S}_i \hat{S}_{i+1} - g\mu_B B_0 \sum_{i=1}^{N} \hat{S}_i$$

Using the definition of partition function ():

$$\begin{aligned} Z_N &= Tr(e^{-\beta H}) \\ &= \sum_{S_1, S_2, \ldots, S_N} e^{\beta \sum_i (g\mu_B B_0 S_i + J S_i S_{i+1})} \\ &= \sum_{S_1, S_2, \ldots, S_N} e^{\beta (g\mu_B B_0 S_1 + J S_1 S_2) + \beta (g\mu_B B_0 S_2 + J S_2 S_3) + \ldots + (g\mu_B B_0 S_N + J S_N S_{N+1})} \\ &= \sum_{S_1, S_2, \ldots, S_N} e^{\beta \left(\frac{1}{2} g\mu_B B_0 (S_1 + S_2) + J S_1 S_2\right) + \beta \left(\frac{1}{2} g\mu_B B_0 (S_2 + S_3) + J S_2 S_3\right) + \ldots + \left(\frac{1}{2} g\mu_B B_0 (S_N + S_1) + J S_N S_{N+1}\right)} \end{aligned}$$

This rearrangement will prove to be useful. Now we want to use the periodic boundary condition $\hat{S}_{N+1} = \hat{S}_1$ and we further define the function:

$$\tau(S_i, S_{i+1}) = \exp\left[\beta \left(J S_i S_{i+1} + \frac{1}{2} g\mu_B B_0 (S_i + S_{i+1})\right)\right]$$

which leads us directly to:

$$\begin{aligned} Z_N &= \sum_{S_1, S_2, \ldots, S_N} e^{\beta \sum_i (g\mu_B B_0 S_i + J S_i S_{i+1})} \\ &= \sum_{S_1, S_2, \ldots, S_N} e^{\beta \left(\frac{1}{2} g\mu_B B_0 (S_1 + S_2) + J S_1 S_2\right) + \beta \left(\frac{1}{2} g\mu_B B_0 (S_2 + S_3) + J S_2 S_3\right) + \ldots + \left(\frac{1}{2} g\mu_B B_0 (S_N + S_1) + J S_N S_1\right)} \\ &= \sum_{S_1, S_2, \ldots, S_N} \tau(S_1, S_2)\, \tau(S_2, S_3) \ldots \tau(S_N, S_1) \end{aligned}$$

b)

The Transfermatix is defined with:

$$T = \begin{pmatrix} \tau\left(\frac{1}{2},\frac{1}{2}\right) & \tau\left(-\frac{1}{2},\frac{1}{2}\right) \\ \tau\left(\frac{1}{2},-\frac{1}{2}\right) & \tau\left(-\frac{1}{2},-\frac{1}{2}\right) \end{pmatrix}$$

this follows from the 4 possible spin combinations, which every S_i, S_{i+1} can have.

We are meant to show, that

$$\sum_{S_i,S_j,S_k} \tau\left(S_i,S_j\right)\tau\left(S_j,S_k\right) = \sum_{S_i,S_j} \left(T^2\right)_{S_i,S_k}$$

with $\left(T^2\right)_{S_i,S_k} = \sum_{S_j} \tau\left(S_i,S_j\right)\tau\left(S_j,S_k\right)$. We can simply write:

$$\begin{aligned} \sum_{S_i,S_j,S_k} \tau\left(S_i,S_j\right)\tau\left(S_j,S_k\right) &= \sum_{S_j}\sum_{S_i,S_k} \tau\left(S_i,S_j\right)\tau\left(S_j,S_k\right) \\ &= \sum_{S_i,S_j} \left(T^2\right)_{S_i,S_k} \end{aligned}$$

c)

We can define the spin states

$$\begin{aligned} |S_i = \frac{1}{2}\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ |S_i = -\frac{1}{2}\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned}$$

and with those we get:

$$\begin{aligned} \left\langle \frac{1}{2}|T| - \frac{1}{2} \right\rangle &= \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} \tau\left(\frac{1}{2},\frac{1}{2}\right) & \tau\left(\frac{1}{2},-\frac{1}{2}\right) \\ \tau\left(\frac{1}{2},-\frac{1}{2}\right) & \tau\left(-\frac{1}{2},-\frac{1}{2}\right) \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ &= \tau\left(\frac{1}{2}, -\frac{1}{2}\right) \end{aligned}$$

or generally

$$\langle S_i|T|S_{i+1}\rangle = \tau\left(S, S_{i+1}\right)$$

This can be inserted in the partition function:

$$\begin{aligned} Z_N &= \sum_{S_1,S_2,\ldots,S_N} \tau\left(S_1,S_2\right)\tau\left(S_2,S_3\right)\ldots\tau\left(S_N,S_1\right) \\ &= \sum_{S_1,S_2,\ldots,S_N} \langle S_1|T|S_2\rangle\langle S_2|T|S_3\rangle\ldots\langle S_N|T|S_1\rangle \end{aligned}$$

using $\sum_{S_i} |S_i\rangle\langle S_i| = 1$ (Vollständigkeit) this leads to:

$$
\begin{aligned}
Z_N &= \sum_{S_1} \langle S_1 | T^N | S_1 \rangle \\
&= Tr\left(T^N\right)
\end{aligned}
$$

the trace definition. While the trace is the sum of the eigenvalues of a matrix and this one is 2x2 we get two different eigenvalues $\lambda_{1,2}$ for T, using the multiplicity this leads to

$$
Z_N = Tr\left(T^N\right) = \lambda_1^N + \lambda_2^N
$$

□

To get the eigenvalues of T, we first write T in full form:

$$
T = \begin{pmatrix} \exp\left[\beta\left(\frac{J}{4} + \frac{1}{2} g\mu_B B_0\right)\right] & \exp\left[\beta\left(-\frac{J}{4}\right)\right] \\ \exp\left[\beta\left(-\frac{J}{4}\right)\right] & \exp\left[\beta\left(\frac{J}{4} - \frac{1}{2} g\mu_B B_0\right)\right] \end{pmatrix}
$$

Calculating the eigenvalues $\lambda_{1,2}$ of the transfer matrix

$$
\det|T - \lambda E| = 0 = \begin{vmatrix} \exp\left[\beta\left(\frac{J}{4} + \frac{1}{2} g\mu_B B_0\right)\right] - \lambda & \exp\left[\beta\left(-\frac{J}{4}\right)\right] \\ \exp\left[\beta\left(-\frac{J}{4}\right)\right] & \exp\left[\beta\left(\frac{J}{4} - \frac{1}{2} g\mu_B B_0\right)\right] - \lambda \end{vmatrix}
$$

leading to

$$
\begin{aligned}
0 &= \left(\exp\left[\beta\left(\frac{J}{4} - \frac{1}{2} g\mu_B B_0\right)\right] - \lambda\right)\left(\exp\left[\beta\left(\frac{J}{4} + \frac{1}{2} g\mu_B B_0\right)\right] - \lambda\right) - \exp\left[2\beta\left(-\frac{J}{4}\right)\right] \\
0 &= \exp\left[\frac{\beta J}{2}\right] - \lambda \exp\left[\beta\left(\frac{J}{4} - \frac{1}{2} g\mu_B B_0\right)\right] - \lambda \exp\left[\beta\left(\frac{J}{4} + \frac{1}{2} g\mu_B B_0\right)\right] + \lambda^2 - \exp\left[-\frac{\beta J}{2}\right] \\
0 &= \lambda^2 - \lambda \exp\left(\frac{\beta J}{4}\right)\left(\exp\left[\frac{\beta}{2} g\mu_B B_0\right] + \exp\left[-\frac{\beta}{2} g\mu_B B_0\right]\right) + \exp\left[\frac{\beta J}{2}\right] - \exp\left[-\frac{\beta J}{2}\right] \\
0 &= \lambda^2 - 2\exp\left(\frac{\beta J}{4}\right)\cosh\left(\frac{\beta}{2} g\mu_B B_0\right)\lambda + 2\sinh\left[\frac{\beta J}{2}\right]
\end{aligned}
$$

meaning the eigenvalues are:

$$
\begin{aligned}
\lambda_{1,2} &= \exp\left(\frac{\beta J}{4}\right)\cosh\left(\frac{\beta}{2} g\mu_B B_0\right) \pm \sqrt{\exp\left(\frac{\beta J}{2}\right)\cosh^2\left(\frac{\beta}{2} g\mu_B B_0\right) - 2\sinh\left[\frac{\beta J}{2}\right]} \\
\lambda_{1,2} &= \exp\left(\frac{\beta J}{4}\right)\left(\cosh\left(\frac{\beta}{2} g\mu_B B_0\right) \pm \sqrt{\cosh^2\left(\frac{\beta}{2} g\mu_B B_0\right) - 2\exp\left(-\frac{\beta J}{2}\right)\sinh\left[\frac{\beta J}{2}\right]}\right)
\end{aligned}
$$

d)

We are considering the limit $\frac{\lambda_2}{\lambda_1} \ll 1$ which means $\lambda_1 \gg \lambda_2$, meaning we can neglect λ_2 and only need to consider λ_1. Using from **c)**

$$
\begin{aligned}
Z_N(T,B_0) &= \lambda_1^N + \lambda_2^N \\
&\approx \lambda_1^N \\
&= \left[\exp\left(\frac{\beta J}{4}\right)\left(\cosh\left(\frac{\beta}{2}g\mu_B B_0\right) + \sqrt{\cosh^2\left(\frac{\beta}{2}g\mu_B B_0\right) - 2\exp\left(-\frac{\beta J}{2}\right)\sinh\left[\frac{\beta J}{2}\right]}\right)\right]^N
\end{aligned}
$$

Definition of free energy:

$$
\begin{aligned}
F(T,B_0) &= -k_B T \ln Z_N(T,B_0) \\
&= -N\frac{J}{4}\ln\left(\cosh\left(\frac{\beta}{2}g\mu_B B_0\right) + \sqrt{\cosh^2\left(\frac{\beta}{2}g\mu_B B_0\right) - 2\exp\left(-\frac{\beta J}{2}\right)\sinh\left[\frac{\beta J}{2}\right]}\right)
\end{aligned}
$$

We can look at special cases $\beta \to \infty$, meaning $T \to 0$ therefore the exponentialterm will vanish and we get:

$$
\begin{aligned}
F(T,B_0) &= -N\frac{J}{4}\ln\left(\cosh\left(\frac{\beta}{2}g\mu_B B_0\right) + \cosh\left(\frac{\beta}{2}g\mu_B B_0\right)\right) \\
&= -N\frac{J}{4}\ln\left(2\cosh\left(\frac{\beta}{2}g\mu_B B_0\right)\right) \\
&= -N\frac{J}{4}\left(\ln 2 + \ln\left[\cosh\left(\frac{\beta}{2}g\mu_B B_0\right)\right]\right)
\end{aligned}
$$

Or the other special case $B_0 \to 0$, we then get using only first order taylor-expansion ($\cosh(x) = 1 + \frac{x^2}{2} + \ldots$):

$$
\begin{aligned}
Z_N(T,0) &\approx \left[\exp\left(\frac{\beta J}{4}\right)\left(1 + \sqrt{1 - 2\exp\left(-\frac{\beta J}{2}\right)\sinh\left[\frac{\beta J}{2}\right]}\right)\right]^N \\
&= \left[\exp\left(\frac{\beta J}{4}\right)\left(1 + \sqrt{1 - \exp\left(-\frac{\beta J}{2}\right)\left[\exp\left(\frac{\beta J}{2}\right) - \exp\left(-\frac{\beta J}{2}\right)\right]}\right)\right]^N \\
&= \left[\exp\left(\frac{\beta J}{4}\right)\left(1 + \sqrt{1 - 1 + \exp(-\beta J)}\right)\right]^N \\
&= \left[\exp\left(\frac{\beta J}{4}\right) + \exp\left(-\frac{\beta J}{4}\right)\right]^N \\
&= \left[2\cosh\left(\frac{\beta J}{4}\right)\right]^N
\end{aligned}
$$

and a free energy of

$$
\begin{aligned}
F(T,0) &= -k_B T \ln Z_N(T,0) \\
&= -N k_B T \ln\left[2\cosh\left(\frac{\beta J}{4}\right)\right]
\end{aligned}
$$

e)

Magnetization:

$$
\begin{aligned}
M(T,B_0) &= \frac{1}{\beta}\left(\frac{\partial}{\partial B_0}\ln Z_N(T,B_0)\right)\\
&= \frac{1}{\beta}\left(\frac{\partial}{\partial B_0}\ln \lambda_1^N\right)\\
&= \frac{N}{\beta}\frac{1}{\lambda_1}\frac{\partial}{\partial B_0}\lambda_1\\
&= \frac{N}{\beta\lambda_1}\exp\left(\frac{\beta J}{4}\right)\frac{\partial}{\partial B_0}\left(\cosh\left(\frac{\beta}{2}g\mu_B B_0\right)+\sqrt{\cosh^2\left(\frac{\beta}{2}g\mu_B B_0\right)-2\exp\left(-\frac{\beta J}{2}\right)\sinh\left[\frac{\beta J}{2}\right]}\right)
\end{aligned}
$$

CAS meaning *mathematica*:

$$
M(T,B_0)=\frac{\beta}{2}g\mu_B\sinh\left(\frac{\beta}{2}g\mu_B B_0\right)\left(1+\frac{\exp\left(-\frac{\beta J}{4}\right)\cosh\left(\frac{\beta}{2}g\mu_B B_0\right)}{\zeta\left(\cosh\left(\frac{\beta}{2}g\mu_B B_0\right)+\zeta\right)}\right)
$$

with $\sqrt{\exp(-\beta J)+\cosh^2\left(\frac{\beta}{2}g\mu_B B_0\right)-1}=\zeta$. While the result of M seems to be wrong we skip the isothermal susceptibility:

$$
\chi_T(B_0)=\frac{\partial M}{\partial B_0}
$$

skipped