4. Plenum aus Statistischer Physik (Lösung)

1. (a) $|x+\rangle$ und $|x-\rangle$ sind die Eigenzustände des Operators $\hat{S}_x$ und $\hat{\sigma}_x$. Wir finden jetzt den Eigenzustand (s,t) von σ_x mit dem Eigenwert λ.

$$\lambda \begin{pmatrix} s \\ t \end{pmatrix} = \sigma_x \begin{pmatrix} s \\ t \end{pmatrix} = \begin{pmatrix} t \\ s \end{pmatrix} \quad \rightarrow \quad s^2 = t^2 \quad \rightarrow \quad t = \pm s$$

Der normierte Vektor $2^{-1/2}(1,1)$ hat den Eigenwert $\lambda = 1$ und $2^{-1/2}(1,-1)$ hat den Eigenwert $\lambda = -1$. Deshalb sind die Spin-up- und -down-Vektoren entlang der x-Achse

$$|x+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |x-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

oder

$$|x+\rangle = \frac{1}{\sqrt{2}} \left(|z+\rangle + |z-\rangle\right), \quad |x-\rangle = \frac{1}{\sqrt{2}} \left(|z+\rangle - |z-\rangle\right).$$

Die Dichtematrix $\hat{\rho}$ in der Basis $\{|x+\rangle, |x-\rangle\}$ ist

$$\rho^X = \begin{pmatrix} \langle x+|\rho|x+\rangle & \langle x+|\rho|x-\rangle \\ \langle x-|\rho|x+\rangle & \langle x-|\rho|x-\rangle \end{pmatrix} = \begin{pmatrix} a & 0 \\ 0 & 1-a \end{pmatrix}$$

(b) Entropie

$$S = -k_B \langle \ln \rho \rangle = -k_B \mathrm{Sp}(\hat{\rho} \ln \hat{\rho})$$

Matrixdarstellung des Operators $\ln \hat{\rho}$:
Wenn die Matrixdarstellung des Operators $\hat{\rho}$ diagonal ist (z.B. ρ^X),

$$\ln \rho^X = \ln \begin{pmatrix} a & 0 \\ 0 & 1-a \end{pmatrix} = \begin{pmatrix} \ln a & 0 \\ 0 & \ln(1-a) \end{pmatrix}$$

und

$$\rho^X \ln \rho^X = \begin{pmatrix} a \ln a & 0 \\ 0 & (1-a)\ln(1-a) \end{pmatrix}.$$

Deshalb ist die Entropie

$$S = -k_B \left(a \ln a + (1-a) \ln(1-a)\right).$$

Das Maximun der Entropie

$$\frac{dS}{da} = -k_B \left(\ln a + 1 - \ln(1-a) - 1\right) = k_B \ln \frac{1-a}{a} = 0\,.$$

Wenn $(1-a)/a = 1$ oder $a = 1/2$, wird die Entropie maximiert.

$$\left.\frac{dS^2}{da^2}\right|_{a=1/2} = k_B \left.\left(-\frac{1}{a} - \frac{1}{1-a}\right)\right|_{a=1/2} = -4k_B < 0$$

2.

Wenn $N = 1$,

Fockzustände :

$$|1,0,0\rangle = |\alpha_1 = -1\rangle$$
$$|0,1,0\rangle = |\alpha_1 = 0\rangle$$
$$|0,0,1\rangle = |\alpha_1 = 1\rangle$$

Kanonische Zustandssumme:

$$\begin{aligned} Z_c &= \langle 1,0,0|e^{-\beta\hat{H}}|1,0,0\rangle + \langle 0,1,0|e^{-\beta\hat{H}}|0,1,0\rangle + \langle 0,0,1|e^{-\beta\hat{H}}|0,0,1\rangle \\ &= e^{-\beta\hbar\gamma B} + 1 + e^{\beta\hbar\gamma B} = 1 + 2\cosh(\beta\hbar\gamma B) \end{aligned}$$

Wenn $N = 2$,

Fockzustände :

$$|2,0,0\rangle = |\alpha_1 = -1, \alpha_2 = -1\rangle$$
$$|0,2,0\rangle = |\alpha_1 = 0, \alpha_2 = 0\rangle$$
$$|0,0,2\rangle = |\alpha_1 = 1, \alpha_2 = 1\rangle$$
$$|1,1,0\rangle = \frac{1}{\sqrt{2}}\left(|\alpha_1 = -1, \alpha_2 = 0\rangle + |\alpha_1 = 0, \alpha_2 = -1\rangle\right)$$
$$|1,0,1\rangle = \frac{1}{\sqrt{2}}\left(|\alpha_1 = -1, \alpha_2 = 1\rangle + |\alpha_1 = 1, \alpha_2 = -1\rangle\right)$$
$$|0,1,1\rangle = \frac{1}{\sqrt{2}}\left(|\alpha_1 = 0, \alpha_2 = 1\rangle + |\alpha_1 = 1, \alpha_2 = 0\rangle\right)$$

Kanonische Zustandssumme:

$$\begin{aligned} Z_c &= \langle 2,0,0|e^{-\beta\hat{H}}|2,0,0\rangle + \langle 0,2,0|e^{-\beta\hat{H}}|0,2,0\rangle + \langle 0,0,2|e^{-\beta\hat{H}}|0,0,2\rangle \\ &\quad + \langle 1,1,0|e^{-\beta\hat{H}}|1,1,0\rangle + \langle 1,0,1|e^{-\beta\hat{H}}|1,0,1\rangle + \langle 0,1,1|e^{-\beta\hat{H}}|0,1,1\rangle \\ &= e^{-2\beta\hbar\gamma B} + 1 + e^{2\beta\hbar\gamma B} + e^{-\beta\hbar\gamma B} + 1 + e^{\beta\hbar\gamma B} \\ &= 2 + 2\cosh(\beta\hbar\gamma B) + 2\cosh(2\beta\hbar\gamma B) \end{aligned}$$

Wenn $N = 3$,

Fockzustände :

$$
\begin{aligned}
|3,0,0\rangle &= |\alpha_1 = -1, \alpha_2 = -1, \alpha_3 = -1\rangle \\
|0,3,0\rangle &= |\alpha_1 = 0, \alpha_2 = 0, \alpha_3 = 0\rangle \\
|0,0,3\rangle &= |\alpha_1 = 1, \alpha_2 = 1, \alpha_3 = 1\rangle \\
|2,1,0\rangle &= \frac{1}{\sqrt{3}} (|\alpha_1 = -1, \alpha_2 = -1, \alpha_3 = 0\rangle + |\alpha_1 = -1, \alpha_2 = 0, \alpha_3 = -1\rangle \\
&\quad + |\alpha_1 = 0, \alpha_2 = -1, \alpha_3 = -1\rangle) \\
|1,2,0\rangle &= \frac{1}{\sqrt{3}} (|\alpha_1 = -1, \alpha_2 = 0, \alpha_3 = 0\rangle + |\alpha_1 = 0, \alpha_2 = -1, \alpha_3 = 0\rangle \\
&\quad + |\alpha_1 = 0, \alpha_2 = 0, \alpha_3 = -1\rangle) \\
|2,0,1\rangle &= \frac{1}{\sqrt{3}} (|\alpha_1 = -1, \alpha_2 = -1, \alpha_3 = 1\rangle + |\alpha_1 = -1, \alpha_2 = 1, \alpha_3 = -1\rangle \\
&\quad + |\alpha_1 = 1, \alpha_2 = -1, \alpha_3 = -1\rangle) \\
|1,0,2\rangle &= \frac{1}{\sqrt{3}} (|\alpha_1 = -1, \alpha_2 = 1, \alpha_3 = 1\rangle + |\alpha_1 = 1, \alpha_2 = -1, \alpha_3 = 1\rangle \\
&\quad + |\alpha_1 = 1, \alpha_2 = 1, \alpha_3 = -1\rangle) \\
|0,2,1\rangle &= \frac{1}{\sqrt{3}} (|\alpha_1 = 0, \alpha_2 = 0, \alpha_3 = 1\rangle + |\alpha_1 = 0, \alpha_2 = 1, \alpha_3 = 0\rangle \\
&\quad + |\alpha_1 = 1, \alpha_2 = 0, \alpha_3 = 0\rangle) \\
|0,1,2\rangle &= \frac{1}{\sqrt{3}} (|\alpha_1 = 0, \alpha_2 = 1, \alpha_3 = 1\rangle + |\alpha_1 = 1, \alpha_2 = 0, \alpha_3 = 1\rangle \\
&\quad + |\alpha_1 = 1, \alpha_2 = 1, \alpha_3 = 0\rangle) \\
|1,1,1\rangle &= \frac{1}{\sqrt{6}} (|\alpha_1 = -1, \alpha_2 = 0, \alpha_3 = 1\rangle + |\alpha_1 = -1, \alpha_2 = 1, \alpha_3 = 0\rangle \\
&\quad + |\alpha_1 = 0, \alpha_2 = -1, \alpha_3 = 1\rangle + |\alpha_1 = 1, \alpha_2 = -1, \alpha_3 = 0\rangle \\
&\quad + |\alpha_1 = 0, \alpha_2 = 1, \alpha_3 = -1\rangle + |\alpha_1 = 1, \alpha_2 = 0, \alpha_3 = -1\rangle)
\end{aligned}
$$

Kanonische Zustandssumme:

$$
\begin{aligned}
Z_c &= e^{-3\beta\hbar\gamma B} + 1 + e^{3\beta\hbar\gamma B} + e^{-2\beta\hbar\gamma B} + e^{-\beta\hbar\gamma B} + e^{-\beta\hbar\gamma B} + e^{\beta\hbar\gamma B} + e^{\beta\hbar\gamma B} + e^{2\beta\hbar\gamma B} + 1 \\
&= 2 + 4\cosh(\beta\hbar\gamma B) + 2\cosh(2\beta\hbar\gamma B) + 2\cosh(3\beta\hbar\gamma B)
\end{aligned}
$$

When $N > 3$, Kanonische Zustandssumme:

$$
\begin{aligned}
Z_c &= \sum_{N_{-1}=0}^{N} \sum_{N_0=0}^{N-N_{-1}} \sum_{N_{+1}=N-N_{-1}-N_0}^{N-N_{-1}-N_0} \langle N_{-1}, N_0, N_{+1} | e^{-\beta \hat{H}} | N_{-1}, N_0, N_{+1} \rangle \\
&= \sum_{N_{-1}=0}^{N} \sum_{N_0=0}^{N-N_{-1}} \sum_{N_{+1}=N-N_{-1}-N_0}^{N-N_{-1}-N_0} \exp\left[\beta \hbar \gamma B \left(-N_{-1} + 0 \times N_0 + N_{+1}\right)\right] \\
&= \sum_{N_{-1}=0}^{N} \sum_{N_0=0}^{N-N_{-1}} \exp\left[\beta \hbar \gamma B \left(-N_{-1} + (N - N_{-1} - N_0)\right)\right] \\
&= \sum_{N_{-1}=0}^{N} \exp\left[\beta \hbar \gamma B \left(-N_{-1} + (N - N_{-1})\right)\right] \frac{1 - \exp(-\beta \hbar \gamma B (N - N_{-1} + 1)}{1 - \exp(-\beta \hbar \gamma B)} \\
&= \sum_{N_{-1}=0}^{N} \frac{\exp(\beta \hbar \gamma B (N - 2N_{-1})) - \exp(\beta \hbar \gamma B (-N_{-1} - 1))}{1 - \exp(-\beta \hbar \gamma B)} \\
&= \frac{1}{1 - e^{-\beta \hbar \gamma B}} \left[e^{\beta \hbar \gamma B N} \frac{1 - e^{-2\beta \hbar \gamma B (N+1)}}{1 - e^{-2\beta \hbar \gamma B}} - e^{-\beta \hbar \gamma B} \frac{1 - e^{-\beta \hbar \gamma B (N+1)}}{1 - e^{-\beta \hbar \gamma B}} \right]
\end{aligned}
$$

Grosskanonische Zustandssumme:

$$
\begin{aligned}
Z_{\mathrm{GK}} &= \sum_{N=0}^{\infty} \sum_{N_{-1}=0}^{N} \sum_{N_0=0}^{N-N_{-1}} \sum_{N_{+1}=N-N_{-1}-N_0}^{N-N_{-1}-N_0} \langle N_{-1}, N_0, N_{+1} | e^{-\beta(\hat{H}-\mu\hat{N})} | N_{-1}, N_0, N_{+1} \rangle \\
&= \sum_{N_{-1}=0}^{\infty} \sum_{N=N_{-1}}^{\infty} \sum_{N_0=0}^{N-N_{-1}} \sum_{N_{+1}=N-N_{-1}-N_0}^{N-N_{-1}-N_0} \langle N_{-1}, N_0, N_{+1} | e^{-\beta(\hat{H}-\mu\hat{N})} | N_{-1}, N_0, N_{+1} \rangle \\
&= \sum_{N_{-1}=0}^{\infty} \sum_{N_0=0}^{\infty} \sum_{N=N_{-1}+N_0}^{\infty} \sum_{N_{+1}=N-N_{-1}-N_0}^{N-N_{-1}-N_0} \langle N_{-1}, N_0, N_{+1} | e^{-\beta(\hat{H}-\mu\hat{N})} | N_{-1}, N_0, N_{+1} \rangle \\
&= \sum_{N_{-1}=0}^{\infty} \sum_{N_0=0}^{\infty} \sum_{N_{+1}=0}^{\infty} \sum_{N=N_{-1}+N_0+N_{+1}}^{N_{-1}+N_0+N_{+1}} \langle N_{-1}, N_0, N_{+1} | e^{-\beta(\hat{H}-\mu\hat{N})} | N_{-1}, N_0, N_{+1} \rangle \\
&= \sum_{N_{-1}=0}^{\infty} \sum_{N_0=0}^{\infty} \sum_{N_{+1}=0}^{\infty} \exp\left[\beta\hbar\gamma B\left(-N_{-1} + 0 \times N_0 + N_{+1}\right) + \beta\mu\left(N_{-1} + N_0 + N_{+1}\right)\right] \\
&= \sum_{N_{-1}=0}^{\infty} \exp\left[-\beta\hbar\gamma B N_{-1} + \beta\mu N_{-1}\right] \sum_{N_0=0}^{\infty} \exp\left[\beta\mu N_0\right] \sum_{N_{+1}=0}^{\infty} \exp\left[\beta\hbar\gamma B N_{+1} + \beta\mu N_{+1}\right] \\
&= \frac{1}{1 - e^{-\beta\hbar\gamma B + \beta\mu}} \frac{1}{1 - e^{\beta\mu}} \frac{1}{1 - e^{\beta\hbar\gamma B + \beta\mu}}
\end{aligned}
$$