

2. Test - Lösungen

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2 M-Niveausystem

a) Alle antisymmetrisierten Permutationen:

$$|\Psi\rangle = |1, 1, 1, 0, 0, \dots\rangle = c(|1\rangle \otimes |2\rangle \otimes |3\rangle - |1\rangle \otimes |3\rangle \otimes |2\rangle + |3\rangle \otimes |1\rangle \otimes |2\rangle - |3\rangle \otimes |2\rangle \otimes |1\rangle + |2\rangle \otimes |3\rangle \otimes |1\rangle - |2\rangle \otimes |1\rangle \otimes |3\rangle).$$

Mit $\langle\Psi|\Psi\rangle = 1 = c^2 \times 6$ folgt $c = 1/\sqrt{6}$.

b) Großkanonische Zustandssumme:

$$\begin{aligned} Z_{GK} &= \text{tr} \left(e^{-\beta(\hat{H} - \mu\hat{N})} \right) \\ &= \sum_{n_1=0}^1 \sum_{n_2=0}^1 \cdots \sum_{n_M=0}^1 \langle n_1, n_2, \dots, n_M | e^{-\beta(\hat{H} - \mu\hat{N})} | n_1, n_2, \dots, n_M \rangle \\ &= \sum_{n_1=0}^1 \sum_{n_2=0}^1 \cdots \sum_{n_M=0}^1 e^{-\beta \sum_{i=1}^M (\epsilon_i n_i - \mu n_i)} \underbrace{\langle n_1, n_2, \dots, n_M | n_1, n_2, \dots, n_M \rangle}_{=1} \\ &= \sum_{n_1=0}^1 \sum_{n_2=0}^1 \cdots \sum_{n_M=0}^1 \left[\prod_{i=1}^M e^{-\beta(\epsilon_i - \mu)n_i} \right] \\ &= \prod_{i=1}^M \left[\sum_{n=0}^1 e^{-\beta(\epsilon_i - \mu)n} \right] \\ &= \prod_{i=1}^M \left[1 + e^{-\beta(\epsilon_i - \mu)} \right]. \end{aligned}$$

c) Großkanonisches Potential:

$$J = -k_B T \ln Z_{GK} = -k_B T \sum_{i=1}^M \ln \left(1 + e^{-\beta(\epsilon_i - \mu)} \right).$$

Entropie:

$$\begin{aligned} S &= - \left. \frac{\partial J}{\partial T} \right|_{V, \mu} \\ &= k_B \sum_{i=1}^M \ln \left(1 + e^{-\beta(\epsilon_i - \mu)} \right) + k_B T \sum_{i=1}^M \frac{e^{-\beta(\epsilon_i - \mu)}}{1 + e^{-\beta(\epsilon_i - \mu)}} \frac{+1}{k_B T^2} (\epsilon_i - \mu) \\ &= k_B \sum_{i=1}^M \left[\ln \left(1 + e^{-\beta(\epsilon_i - \mu)} \right) + \frac{1}{k_B T} \frac{\epsilon_i - \mu}{e^{\beta(\epsilon_i - \mu)} + 1} \right]. \end{aligned}$$

Für $T \rightarrow \infty$ geht $\beta = 1/(k_B T) \rightarrow 0$.

$$\lim_{T \rightarrow \infty} S = k_B \sum_{i=1}^M \left[\ln(1 + e^0) + 0 \frac{\epsilon_i - \mu}{e^0 + 1} \right] = k_B \sum_{i=1}^M \ln 2 = M k_B \ln 2.$$

Für $M = 5$ folgt $\lim_{T \rightarrow \infty} S = 5 \ln 2$.

3 Asymmetrische harmonische Falle

$$H = \frac{p_x^2 + p_y^2}{2m} + \frac{m\omega^2}{2} (a^2 x^2 + b^2 y^2).$$

a) Großkanonische Zustandssumme:

$$\begin{aligned} Z_{GK}(T, V, \mu) &= \sum_{N=0}^{\infty} e^{\beta\mu N} \frac{1}{h^{2N} N!} \int e^{-\beta H(p, q)} d^{2N} p d^{2N} q \\ &= \sum_{N=0}^{\infty} e^{\beta\mu N} \frac{1}{h^{2N} N!} \int e^{-\beta \sum_{i=1}^{2N} \frac{p_i^2}{2m} + \sum_{i=1}^N \left(\frac{ma^2 \omega^2 q_i^2}{2} + \frac{mb^2 \omega^2 q_{N+i}^2}{2} \right)} d^{2N} p d^{2N} q \\ &= \sum_{N=0}^{\infty} \frac{e^{\beta\mu N}}{h^{2N} N!} \left(\prod_{i=1}^{2N} \int_{-\infty}^{\infty} dp_i e^{-\beta \frac{p_i^2}{2m}} \right) \left(\prod_{i=1}^N \int_{-\infty}^{\infty} dq_i e^{-\beta \frac{ma^2 \omega^2 q_i^2}{2}} \right) \left(\prod_{i=N+1}^{2N} \int_{-\infty}^{\infty} dq_i e^{-\beta \frac{mb^2 \omega^2 q_i^2}{2}} \right) \\ &= \sum_{N=0}^{\infty} e^{\beta\mu N} \frac{1}{h^{2N} N!} \left(\int_{-\infty}^{\infty} dp e^{-\beta \frac{p^2}{2m}} \right)^{2N} \left(\int_{-\infty}^{\infty} dq e^{-\beta \frac{ma^2 \omega^2 q^2}{2}} \right)^N \left(\int_{-\infty}^{\infty} dq e^{-\beta \frac{mb^2 \omega^2 q^2}{2}} \right)^N \\ &= \sum_{N=0}^{\infty} e^{\beta\mu N} \frac{1}{h^{2N} N!} \left(\sqrt{\frac{2m\pi}{\beta}} \right)^{2N} \left(\sqrt{\frac{2\pi}{\beta a^2 m \omega^2}} \right)^N \left(\sqrt{\frac{2\pi}{\beta b^2 m \omega^2}} \right)^N \\ &= \sum_{N=0}^{\infty} \frac{1}{N!} \left[e^{\beta\mu} \frac{1}{ab} \left(\frac{2\pi}{h\omega\beta} \right)^2 \right]^N = \exp \left(e^{\beta\mu} \frac{1}{ab} \left(\frac{2\pi}{h\omega\beta} \right)^2 \right) = \exp \left(e^{\frac{\mu}{k_B T}} \frac{1}{ab} \left(\frac{k_B T}{\hbar\omega} \right)^2 \right), \end{aligned}$$

mit $\beta = 1/(k_B T)$ und $\hbar = h/(2\pi)$.

Für $a = 1$ und $b = 4$ folgt

$$Z_{GK}(T, V, \mu) = \exp \left(e^{\beta\mu} \left(\frac{\pi}{h\omega\beta} \right)^2 \right).$$

b) Mittlere Teilchenzahl:

$$\begin{aligned} \langle N \rangle &= \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Z_{GK} \\ &= \frac{1}{\beta} \frac{\partial}{\partial \mu} e^{\beta\mu} \frac{1}{ab} \left(\frac{2\pi}{h\omega\beta} \right)^2 \\ &= e^{\beta\mu} \frac{1}{ab} \left(\frac{2\pi}{h\omega\beta} \right)^2. \end{aligned}$$

Für $a = 1$ und $b = 4$ folgt $\langle N \rangle = e^{\beta\mu} (\pi/h\omega\beta)^2$.

c) Mittlere Energie:

$$\begin{aligned} \langle E \rangle &= - \frac{\partial}{\partial \beta} \ln Z_{GK} \Big|_{z=e^{\beta\mu}} \\ &= -e^{\beta\mu} \frac{\partial}{\partial \beta} \frac{1}{ab} \left(\frac{2\pi}{h\omega\beta} \right)^2 \\ &= -e^{\beta\mu} \frac{1}{ab} \left(\frac{2\pi}{h\omega} \right)^2 \frac{-2}{\beta^3} \\ &= \frac{2}{\beta} \langle N \rangle. \end{aligned}$$

Daher ist $\langle E \rangle / \langle N \rangle = 2/\beta$.