2. Test - Lösungen **17.06.2011**

2 M-Niveausystem

a) Alle antisymmetrisierten Permutationen:

$$\begin{aligned} |\Psi\rangle = |1,1,1,0,0,\ldots\rangle &= c\,(|1\rangle \otimes |2\rangle \otimes |3\rangle - |1\rangle \otimes |3\rangle \otimes |2\rangle + |3\rangle \otimes |1\rangle \otimes |2\rangle \\ &\quad - |3\rangle \otimes |2\rangle \otimes |1\rangle + |2\rangle \otimes |3\rangle \otimes |1\rangle - |2\rangle \otimes |1\rangle \otimes |3\rangle)\,. \end{aligned}$$

Mit $\langle\Psi|\,\Psi\rangle = 1 = c^2 \times 6$ folgt $c = 1/\sqrt{6}$.
b) Großkanonische Zustandssumme:

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

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

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

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

3 Asymmetrische harmonische Falle

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

a) Großkanonische Zustandssumme:

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

mit $\beta = 1/(k_BT)$ und $\hbar = h/(2\pi)$.
Für $a^2 = 1$ und $b^2 = 4$ folgt mit $ab = 2$

$$Z_{GK}(T,V,\mu) = \exp\left(e^{\beta\mu}\frac{1}{2}\left(\frac{2\pi}{h\omega\beta}\right)^2\right).$$

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