6. Rechenübung aus Statistischer Physik (Lösung)

1. (a) Gleichgewicht bei konstanten $(V, T, N) \rightarrow$ kanonisches Ensemble :
   Wahrscheinlichkeitsdichte im Phasenraum

$$\rho(\vec{r}_1, \vec{p}_2, \cdots, \vec{r}_N, \vec{p}_N) = \frac{1}{Z_c} \frac{1}{N! h^{3N}} e^{-\beta \sum_{i=1}^{N} |p_i|^2/(2m)}$$

   Zustandssumme (Normierungsfaktor):

$$\begin{aligned} Z_c(V, T, N) &= \frac{1}{N! h^{3N}} \int e^{-\beta \sum_{i=1}^{N} |p_i|^2/(2m)} d^{3N} r d^{3N} p_r \\ &= \frac{V^N}{N! h^{3N}} \left(\int e^{-\beta p^2/(2m)} dp \right)^{3N} \\ &= \frac{V^N}{N! h^{3N}} \left(\frac{2\pi m}{\beta} \right)^{3N/2} = \frac{1}{N!} \left(\frac{V}{\lambda_T^3} \right)^N \end{aligned}$$

   wobei $\lambda = h/\sqrt{2\pi m k_B T}$.

   (b) Wahrscheinlichkeit :

$$\begin{aligned} P(N_1) &= \frac{1}{Z_c} \underbrace{\frac{N!}{N_1!(N-N_1)!}}_{\substack{\text{Auswahl von } N_1 \\ \text{aus } N \text{ Teilchen}}} \int d^{3N} p_r \underbrace{\int_{V_1} d^{3N_1} r}_{\substack{N_1 \text{ Teilchen} \\ \text{in } V_1}} \underbrace{\int_{V-V_1} d^{3(N-N_1)} r}_{\substack{N-N_1 \text{ Teilchen} \\ \text{in } V-V_1}} \rho \\ &= \frac{1}{Z_c} \frac{N!}{N_1!(N-N_1)!} \frac{1}{N!} \frac{V_1^{N_1} (V-V_1)^{N-N_1}}{\lambda_T^{3N}} \\ &= \frac{N!}{N_1!(N-N_1)!} \frac{V_1^{N_1} (V-V_1)^{N-N_1}}{V^N} \\ &= \frac{N!}{N_1!(N-N_1)!} \gamma^{N_1} (1-\gamma)^{N-N_1} \end{aligned}$$

   $(\gamma = V_1/V)$.

   (c)

$$\begin{aligned} \langle N_1 \rangle &= \sum_{N_1=0}^{N} N_1 P(N_1) \\ &= \sum_{N_1=1}^{N} \frac{N!}{(N_1-1)!(N-N_1)!} \gamma^{N_1} (1-\gamma)^{N-N_1} \\ &= N\gamma \underbrace{\sum_{N_1=1}^{N} \frac{(N-1)!}{(N_1-1)!(N-N_1)!} \gamma^{N_1-1} (1-\gamma)^{N-N_1}}_{=1} \\ &= N \frac{V_1}{V} \end{aligned}$$

$$P(N_1) = \frac{N!}{N_1!(N-N_1)!} \gamma^{N_1} (1-\gamma)^{N-N_1}$$

$$
\begin{aligned}
&= \frac{N!}{N_1!(N-N_1)!}\left(\frac{\langle N_1\rangle}{N}\right)^{N_1}\left(1-\frac{\langle N_1\rangle}{N}\right)^{N-N_1} \\
&= \frac{N!}{N^{N_1}(N-N_1)!}\frac{\langle N_1\rangle^{N_1}}{N_1!}\left[\left(1-\frac{\langle N_1\rangle}{N}\right)^{N/\langle N_1\rangle}\right]^{\langle N_1\rangle(N-N_1)/N} \\
&\rightarrow \frac{\langle N_1\rangle^{N_1}}{N_1!}e^{-\langle N_1\rangle}
\end{aligned}
$$

Zusätzliche Information:
Reduzierte Verteilungsfunktion, die im Volumen V_1 normiert wird

$$
\begin{aligned}
& \rho(\vec{r}_1,\vec{p}_1,\cdots,\vec{r}_{N_1},\vec{p}_{N_1},N_1) \\
=\ & P(N_1)\left(\frac{V}{V_1}\right)^{N_1}\int\rho(\vec{r}_1,\vec{p}_1,\cdots,\vec{r}_N,\vec{p}_N)d^{N-N_1}rd^{N-N_1}p \\
=\ & P(N_1)\left(\frac{V}{V_1}\right)^{N_1}\frac{1}{Z_c}\frac{1}{N!h^{3N_1}}\left(\frac{V}{\lambda_T^3}\right)^{N-N_1}e^{-\beta\sum_{i=1}^{N_1}|p_i^2|/(2m)} \\
=\ & P(N_1)\left(\frac{V}{V_1}\right)^{N_1}\frac{1}{h^{3N_1}}\left(\frac{V}{\lambda_T^3}\right)^{-N_1}e^{-\beta\sum_{i=1}^{N_1}|p_i^2|/(2m)} \\
=\ & \frac{\langle N_1\rangle^{N_1}}{N_1!}e^{-\langle N_1\rangle}\frac{1}{h^{3N_1}}\left(\frac{\lambda_T^3}{V_1}\right)^{N_1}e^{-\beta\sum_{i=1}^{N_1}|p_i^2|/(2m)} \\
& \left(\text{Chemisches Potential}: \ \mu = k_BT\ln\frac{\langle N_1\rangle\lambda_T^3}{V_1}\right) \\
=\ & \frac{1}{N_1!h^{3N_1}}\left(e^{\beta\mu}\frac{V_1}{\lambda_T^3}\right)^{N_1}\exp\left(-e^{\beta\mu}\frac{V_1}{\lambda_T^3}\right)\left(\frac{\lambda_T^3}{V_1}\right)^{N_1}e^{-\beta\sum_{i=1}^{N_1}|p_i^2|/(2m)} \\
=\ & \frac{1}{N_1!h^{3N_1}}\exp\left(-e^{\beta\mu}\frac{V_1}{\lambda_T^3}\right)e^{-\beta\left(\sum_{i=1}^{N_1}|p_i^2|/(2m)-N_1\mu\right)} \\
\rightarrow\ & \text{großkanonische Verteilung}
\end{aligned}
$$

2. (a) Gleichgewicht bei konstanten $(T,\mu,\omega)\rightarrow$ großkanonisches Ensemble
Zustandssumme:

$$
\begin{aligned}
Z_{\text{GK}} &= \sum_{N=0}^{\infty}\frac{1}{N!h^{3N}}e^{\beta\mu N}\int d^{3N}rd^{3N}pe^{-\beta H} \\
&= \sum_{N=0}^{\infty}\frac{1}{N!h^{3N}}e^{\beta\mu N}\left(\int dre^{-\beta m\omega^2r^2/2}\right)^{3N}\left(\int dre^{-\beta p^2/(2m)}\right)^{3N} \\
&= \sum_{N=0}^{\infty}\frac{1}{N!h^{3N}}e^{\beta\mu N}\left(\frac{2\pi k_BT}{m\omega^2}\right)^{3N/2}(2\pi mk_BT)^{3N/2} \\
&= \sum_{N=0}^{\infty}\frac{1}{N!}\left(\left(\frac{k_BT}{\hbar\omega}\right)^3e^{\beta\mu}\right)^N \\
&= \exp\left[\left(\frac{k_BT}{\hbar\omega}\right)^3e^{\beta\mu}\right]
\end{aligned}
$$

(b)

$$
\langle N\rangle = \frac{1}{Z_{\text{GK}}}\sum_{N=0}^{\infty}N\frac{1}{N!h^{3N}}e^{\beta\mu N}\int d^{3N}rd^{3N}pe^{-\beta H}
$$

$$
\begin{aligned}
&= \frac{1}{\beta}\frac{1}{Z_{\mathrm{GK}}}\frac{\partial}{\partial\mu}\sum_{N=0}^{\infty}\frac{1}{N!h^{3N}}e^{\beta\mu N}\int d^{3N}r d^{3N}p e^{-\beta H} \\
&= \frac{1}{\beta}\frac{1}{Z_{\mathrm{GK}}}\frac{\partial}{\partial\mu}Z_{\mathrm{GK}} \\
&= \frac{1}{\beta}\frac{\partial}{\partial\mu}\ln Z_{\mathrm{GK}} \\
&= \left(\frac{k_B T}{\hbar\omega}\right)^3 e^{\beta\mu}
\end{aligned}
$$

(c)

$$
\begin{aligned}
P(N) &= \frac{1}{Z_{\mathrm{GK}}}\frac{1}{N!h^{3N}}e^{\beta\mu N}\int d^{3N}r d^{3N}p e^{-\beta H} \\
&= \frac{1}{Z_{\mathrm{GK}}}\frac{1}{N!}\left(\left(\frac{k_B T}{\hbar\omega}\right)^3 e^{\beta\mu}\right)^N \\
&= e^{-\langle N\rangle}\frac{1}{N!}\langle N\rangle^N
\end{aligned}
$$