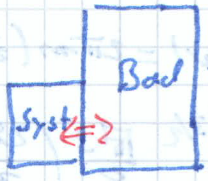
TUS-Übung

18.12.18

mikrokan. Ensemble

kein Austausch
→ E konstant
→ $N, V = \text{const}$

kan. Ensemble

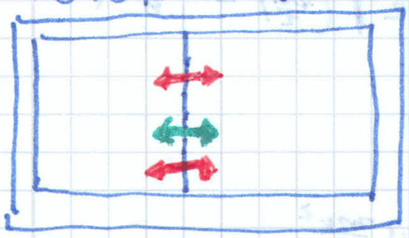


⟺ Wärmeaustausch
→ T const, E nicht mehr
→ N, V const

$Z_{kan}(T,N,V) \sim \int d^{3N}p\, d^{3N}q\, e^{-\beta H(p,q)}$

theoretisch alle Integrale von $-\infty$ bis ∞ aber $H(p,q) = \infty$ außerhalb der Systemwände

Großkan.



⟷ Teilchenaustausch
→ T, V const

⟷ Wärmeaustausch
→ N nicht mehr const, sondern μ

$$Z_{Gr} = Z_{Gr}(T,V,\mu) = \sum_{N=0}^{\infty} \underbrace{e^{\beta\mu N}}_{\text{Fugazität}} Z_{kan}(T,V,N)$$

Aufgabe 2)

$$H = \frac{p^2}{2m} + V(\vec{q}) \qquad V(\vec{q}) = c(|x|+|y|+|z|)$$

$$\rho = (\vec{q},\vec{p}) = \frac{1}{Z} e^{-\beta H}$$

$$1 \overset{!}{=} \int d^3p \int d^3q\, \frac{1}{Z} e^{-\beta H} = \frac{1}{Z} \int d^3p\, e^{-\beta \frac{p^2}{2m}} \int d^3q\, e^{-\beta c(|x|+|y|+|z|)}$$

$$Z = \underbrace{\left(\int dp\, e^{-\beta\frac{p^2}{2m}}\right)^3}_{\frac{h^3}{\lambda^3}} \left(2\int_0^a dx\, e^{-\beta c x}\right)^3 = \frac{h^3}{\lambda^3}\left(\frac{2}{\beta c}\left(1-e^{-\beta c a}\right)\right)^3$$

$$\rho(\vec{q},\vec{p}) = \frac{1}{Z} 4\pi p^2 e^{-\beta H}$$

$$n(v,\vec{q})\,dv = \rho(p,\vec{q})\,dp \rightarrow n(v,\vec{q}) = \rho(\vec{q},\vec{p})\left|\frac{\partial p}{\partial v}\right| = \frac{4\pi m^3 v^2}{Z} e^{-\beta\left(\frac{mv^2}{2}+V\right)}$$

b)

$$n(v) = \int d^3q\, n(v,\vec{q}) = \frac{4\pi m^3 v^2}{Z} e^{-\beta\frac{mv^2}{2}} \int d^3q\, e^{-\beta V}$$

$$= \left(\frac{m}{2\pi k_B T}\right)^{3/2} 4\pi v^2 e^{-\beta\frac{mv^2}{2}}$$

c) $$\langle v\rangle = \int_0^\infty dv\, v\, n(v) = \left(\frac{m}{2\pi k_BT}\right)^{3/2} 4\pi \int dv\, v^3 e^{-\beta\frac{mv^2}{2}} = \ldots = \sqrt{\frac{8k_BT}{\pi m}}$$

$$\langle E\rangle = \frac{m}{2}\int_0^\infty v^2 n(v) = 2\pi m\left(\frac{m}{2\pi k_BT}\right)^{3/2}\int_0^\infty dv\, v^4 e^{-\frac{\beta m v^2}{2}} \quad (1)$$

$$= 2\pi m\left(\frac{m}{2\pi k_BT}\right)^{3/2}\frac{\sqrt{\pi}\,3}{8}\left(\frac{2k_BT}{m}\right)^{5/2} = \underline{\underline{\frac{3}{2}k_BT}}$$

$$NR:\ (1) = \frac{\partial^2}{\partial(\frac{\beta m}{2})^2}\int_0^\infty dv\, e^{-\beta\frac{mv^2}{2}} = \frac{\partial^2}{\partial(\frac{\beta m}{2})^2}\cdot\frac{1}{2}\sqrt{\frac{\pi}{(\frac{\beta m}{2})}} = \frac{\sqrt{\pi}\,3}{8}\left(\frac{2k_BT}{m}\right)^{5/2}$$

$$v(E) = \sqrt{\frac{2E}{m}},\quad E(v) = \frac{1}{2}mv^2$$

d) $$\rho(E) = n(v)\left|\frac{dv}{dE}\right| = \left(\frac{m}{2\pi k_BT}\right)^{3/2} 4\pi v^2 e^{-\beta\frac{mv^2}{2}}\frac{1}{mv}$$

$$= \left(\frac{m}{2\pi k_BT}\right)^{3/2} 4\pi\,\frac{2E}{m^2}\,e^{-\beta E}\frac{1}{\sqrt{\frac{2E}{m}}} = 2\sqrt{\frac{E}{\pi}}\,\beta^{3/2}e^{-\beta E}$$

$$\langle E\rangle = \int_0^\infty dE\, E\rho(E) = \frac{2}{\sqrt{\pi}}\beta^{3/2}\int_0^\infty E^{3/2}e^{-\beta E}$$

$$= \frac{2}{\sqrt{\pi}}\beta^{3/2}\frac{3\sqrt{\pi}}{4\beta^{5/2}} = \frac{3}{2}k_BT$$

3c) es gilt: $$\langle H\rangle - \mu\langle N\rangle = -\frac{\partial}{\partial\beta}\ln(Z_{gk}) = \frac{1}{Z_{gk}}\left(-\frac{\partial Z_{gk}}{\partial\beta}\right)$$

$$-\frac{\partial}{\partial\beta}\ln(Z_{gk}) = -\frac{\partial}{\partial\beta}\left[z\,\frac{8\pi V}{(c\beta h)^3}\right] = -\mu\ln(Z_{gk}) + \frac{3}{\beta}\ln(Z_{gk})$$

$$\boxed{\ln(Z_{gk}) = -\beta\Omega} \qquad = \mu\beta\Omega - 3\Omega = 3pV - \mu\langle N\rangle$$

$$\boxed{\beta\Omega = \frac{\partial\Omega}{\partial\mu}\Big|_{T,V} = -\langle N\rangle}$$