QM Tipps 9

9.1 $\quad \underline{x} = (x_1, \dots, x_N) = (q_1 \dots q_N, p_1, \dots p_N) \in \Gamma$

Kanonisches Ensemble
$$\left\{ \begin{aligned} w(x)\,dx &= \frac{1}{Z(\beta)} e^{-\beta H(x)} \\ Z(\beta) &= \int_\Gamma d\underline{x}\, e^{-\beta H(\underline{x})} \end{aligned} \right.$$

$f : \Gamma \to \mathbb{R}$ "Observable", z.B. $H(\underline{x})$

$$\langle f \rangle_\beta = \int_\Gamma f(\underline{x})\, w(\underline{x})\, d\underline{x} = \int \frac{f(\underline{x}) e^{-\beta H(\underline{x})}}{Z(\beta)}\, d\underline{x}$$

$$S = -k \int w(\underline{x}) \log w(\underline{x})\, d\underline{x} = k\beta \underbrace{\langle H \rangle_\beta}_{= U} + k \log Z(\beta)$$

$$F(\beta) = U - TS = -\frac{1}{\beta} \log Z(\beta)$$

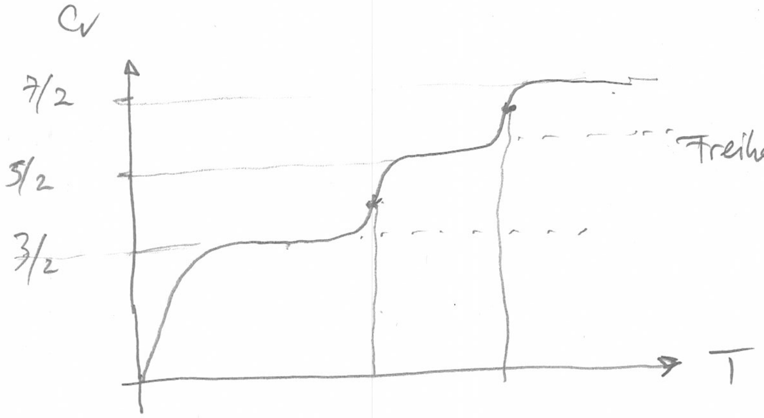
$$U = \langle H \rangle_\beta = -\frac{\partial}{\partial\beta} \log Z(\beta) \qquad c_V = \frac{dU}{dT} = \dots = -\frac{1}{kT^2} \frac{\partial U}{\partial \beta}$$

Quantenstatistik

Sei $A = A^*$ Operator auf $\mathcal{H} = L^2(\mathbb{R}^{3N}, d^{3N}x)$

$$\langle A \rangle = \mathrm{tr}(A P_\beta), \quad P_\beta = \frac{1}{Z(\beta)} e^{-\beta H}, \quad Z(\beta) := \mathrm{tr}\, e^{-\beta H}$$
$$= \sum_n \langle \psi_n, e^{-\beta H} \psi_n \rangle \quad \{\psi_n\} \text{ ONB}$$

notwendig: H hat Punktspektrum

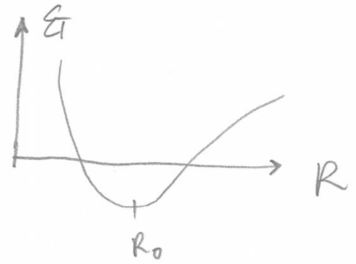


Translat Rot

Freiheitsgrade: 3 + 2 + 1 + 1

Ansatz: $C_V = \frac{3}{2}k + c_V^{vib} + C_V^{rot}$

$$H^{rot} = \frac{\hbar^2 \vec{L}^2}{2\Theta}, \quad \Theta = M_{red} R_0^2 = \mu R_0^2$$



$$EW = \hbar^2 \frac{l(l+1)}{2\Theta}$$

$$\mathrm{tr}\, e^{-\beta H^{rot}} = \sum_\alpha \langle \psi_\alpha, e^{-\beta H^{rot}} \psi_\alpha \rangle$$

Eigenfkt's: $\sim Y_l^m$

$$= \sum_\alpha e^{-\beta \frac{l(l+1)}{2\Theta}} \langle \psi_\alpha, \psi_\alpha \rangle$$

$\alpha = (l, m)$

$$\overset{\text{normiert}}{1 =} \sum_{l,m} e^{-\frac{\beta\hbar^2 l(l+1)}{2\Theta}} = \sum_{l=0}^{\infty} \underbrace{(2l+1)}_{\text{Entartung in } m} e^{-\frac{\beta l(l+1)}{2\Theta}}$$

analytisch nicht berechenbar

Betrachte Grenzwerte $\beta \to 0$, $\beta \to \infty$

$$\sum_{l=0}^{\infty} f(l) \simeq \int_0^\infty f(l)\,dl + \frac{1}{2} f(0) - \frac{1}{12} f'(0) + \dots$$

Euler-Maclaurin

$$(f(0) - f(\infty)) - \frac{1}{12}(f'(0) - f'(\infty))$$

$$H(\phi_{ext}, \vec{A}_{ext}) = \frac{-1}{2m}\left(\vec{p} - e\,A_{ext}\right)^2 - \frac{e^2}{|x|} + e\,\phi_{ext}$$

Dipolapprox: $E(x,t) = E(t)$, kein B-Feld

$$H_K(t) = \frac{-1}{2m}\left(\vec{p} - e\vec{A}(t)\right) - \frac{e^2}{|x|}, \quad A(t) = -\int_{-\infty}^{t} \vec{E}(t')\,dt',$$

$$-A(t) = \vec{E}(t)$$

$$H_R(t) = -\frac{1}{2m}\Delta - \frac{e^2}{|x|} - e\underbrace{E(t)\cdot x}_{\phi(t,x)}, \quad \vec{A} = 0$$

Eichtransformation: $\Lambda(x,t)$

$$\vec{A} \to \tilde{\vec{A}} = \vec{A} + \vec{\nabla}\Lambda$$

$$\phi \to \tilde{\phi} = \phi - \partial_t \Lambda$$

$$\psi \to \tilde{\psi} = e^{+ie\Lambda}\psi$$

Wähle $\Lambda(x,t) = \underline{\underline{-\vec{A}(t)}}\cdot\vec{x}$

H_K: $U_K(t,s)$ s.d. $\psi(t) = U_K(t,s)\psi(s)$

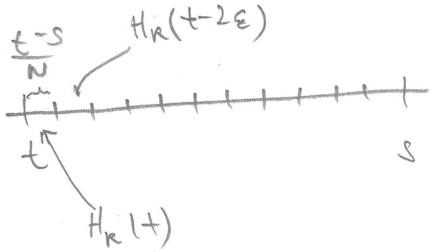
H_R: $U_R(t,s)$ s.d. $\tilde{\psi}(t) = U_R(t,s)\tilde{\psi}(s)$

z.z. $U_K(t,s) = e^{ie\Lambda(x,t)}\,U_R\,e^{-ie\Lambda(x,s)}, \quad \Lambda(x,t) = A(t)\,x$

9.3

$$U_R(t,s) = s\text{-}\lim_{N\to\infty} \prod_{j=1}^{N-1} e^{-i\varepsilon H_R(t-j\varepsilon)}, \quad \varepsilon = \frac{t-s}{N}$$

$\Rightarrow$



$$\underbrace{e^{ie\Lambda(x,t)} e^{-i\varepsilon H_R(t)} e^{-ie\Lambda(x,t)}}\ \underbrace{e^{ie\Lambda(x,t)} e^{-ie\Lambda(x,t-\varepsilon)}}\ e^{ie\Lambda(x,t-\varepsilon)}$$

$$\times e^{-i\varepsilon H_R(t-\varepsilon)}$$

$$e^{ie\Lambda(x,t)-ie\Lambda(x,t-\varepsilon)} = e^{ie\varepsilon\dot{\Lambda}(t)}$$

$$e^{-i\varepsilon H_R(t)} \simeq \mathbb{1} - i\varepsilon H_R(t) + O(\varepsilon^2)$$

QM 1, Aufgabe 4.1

$$e^{-ie\Lambda(x,t)}(\vec{p} - e\vec{A})^2\psi = (\vec{p} - e\vec{A} + e\vec{\nabla}\Lambda)^2 e^{-ie\Lambda(x,t)}\psi$$

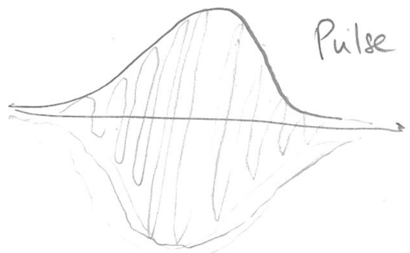
$$\widetilde{(\vec{p} - e\vec{A})^2\psi} = (\underbrace{\vec{p} - e\vec{A} + e\vec{\nabla}A}_{=\,\widetilde{(\vec{p} - e\vec{A})}})^2 \tilde{\psi}$$

$$\Rightarrow e^{-i\varepsilon[-\frac{1}{2m}(\vec{p}-e\vec{A})^2 - e\vec{E}(t)\vec{x} - \frac{e^2}{|x|}]}\ e^{ie\varepsilon E(t)\vec{x}}$$

Bmk: $e^A e^B = e^{\underbrace{A+B}_{O(\varepsilon)} + O(\varepsilon^2)}$

$H(t) = H_0 + V(t) \qquad V(t) = -e\,E(t)\,\vec{x}$

$E(t) = E_0\, e^{-\frac{t^2}{T^2}} \begin{pmatrix} 0 \\ 0 \\ \cos\omega t \end{pmatrix}$



Zeit $\quad s \to -\infty \quad \psi_{nem} \equiv \psi_i$

$\qquad t \to +\infty \quad \psi_{n'e'm'} \equiv \psi_f \qquad P_{fi}^{(2)}(t,s)$

(9.39) $\quad P_{fi}^{(2)}(t,s) = \frac{1}{\hbar^2} \left| \int_s^t dt'\, e^{i\omega_{fi} t'} \langle \psi_f, V(t')\psi_i \rangle \right|^2$

$\omega_{fi} = \frac{E_f - E_i}{\hbar} \qquad \sim \hat{z}$

ii) $\quad P_{fi}^{(2)}(\infty, -\infty)$ mit $\psi_i = \psi_{100}$

$\qquad \psi_f = \psi_{200} \qquad \psi_{100} = \frac{1}{\sqrt{\pi a^3}}\, e^{-\frac{r}{a}}$

$\langle \psi_{100}, z\,\psi_{210} \rangle = \frac{2^8}{3^5\sqrt{2}} \cdot a \quad , \quad \int_{-\infty}^{\infty} dx\, e^{ik\vec{x}}\, e^{-x^2/c^2} = 2\frac{\sqrt{\pi}}{c}\, e^{-\frac{k^2c^2}{4}}$

Vereinfache:

Einlaufendes Teilchen: $e^{-i\frac{\vec{p}}{\hbar}\vec{x}} \qquad \vec{E} = E_0 \cos(\omega t)\,\hat{z}$

$P_{fi}^{(2)}(\infty, -\infty) = \langle e^{-i\frac{\vec{p}}{\hbar}\vec{x}}, \hat{V}(\omega_{fi})\, e^{-\frac{r}{a}} \rangle \cdot \text{const}$

$\vec{k} = \frac{\vec{p}}{\hbar} \quad \rightsquigarrow \quad \langle e^{-ik\vec{x}}, z\, e^{-\frac{r}{a}} \rangle$