

Wdh

$$|\psi\rangle = -\frac{i}{\hbar} H |\psi\rangle \rightsquigarrow |\psi(t)\rangle = U(t) |\psi_0\rangle$$

$$\rightsquigarrow \dot{U}(t) = -\frac{i}{\hbar} H U(t) \rightsquigarrow U^{\dagger}(t) = +\frac{i}{\hbar} U^{\dagger}(t) H(t)$$

$$\rho = |\psi(t)\rangle \langle \psi(t)| = U(t) |\psi_0\rangle \langle \psi_0| U^{\dagger}(t)$$

$$\dot{\rho} = -\frac{i}{\hbar} H(t) \rho(t) + \rho(t) \left(+\frac{i}{\hbar} H(t)\right) \rightsquigarrow \frac{i}{\hbar} [H(t), \rho]$$

• DM $\{|\Phi_i\rangle\}$ $\langle \Phi_i | \Phi_j \rangle = \delta_{ij}$

$$0 \leq P_i \leq 1 \quad \sum_i P_i = 1 \quad \rho = \sum_i P_i |\Phi_i\rangle \langle \Phi_i|$$

jede DM erfüllt $\text{Tr}\{\rho\} = 1$

$$\rho = \rho^{\dagger}$$

ρ ist positiv semidefinit

$$\langle \psi | \rho | \psi \rangle \geq 0$$

EW von ρ
 \downarrow
 $P_i \geq 0$

$$\text{Tr}\{\rho\} = \sum_i P_i \text{Tr}\{|\Phi_i\rangle \langle \Phi_i|\} = \sum_i P_i = 1$$

$$\langle \psi | \rho | \psi \rangle = \sum_i P_i \langle \psi | \Phi_i\rangle \langle \Phi_i | \psi \rangle = \sum_i P_i |\langle \psi | \Phi_i \rangle|^2 \geq 0$$

• Quanten-Messung für diskrete MS-Wert P_i

$$\text{ERW} \quad \left[\begin{aligned} \langle A \rangle &= \text{Tr}\{A \rho\} \\ &= \text{Tr}\{\rho A\} \end{aligned} \right] = \sum_i P_i \langle \Phi_i | A | \Phi_i \rangle$$

• "reine" Zustände

$$\rho^2 = \rho$$

$$\rho = (1 \times 1)$$

z.B. $\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

"gemischte"

: Gemischt $\rho^2 \neq \rho$

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = (1 \times 1)$$

$$|1\rangle = \frac{1}{\sqrt{2}} [|0\rangle + |1\rangle]$$

• Messprozess: $\{M_n\}$: $\sum_n M_n^{\dagger} M_n = \mathbb{1}$

projektive Messung $M_n \rightarrow 1 \times 1$

$$\rho \xrightarrow{(n)} \frac{M_n \rho M_n^{\dagger}}{P_n} \quad P_n = \text{Tr}\{M_n \rho M_n^{\dagger}\} = \text{Tr}\{M_n^{\dagger} M_n \rho\}$$

- "Populationen": Diagonalelemente von ρ
- "Kohärenzen": Off-Diagonalelemente

} basis-abhängig

3.1.3. Allgemeine Entwicklung

$$\left[\text{Kronecker-Abb.: } \rho' = \sum_k k_x \rho k_x^\dagger \quad \sum_k k_x^\dagger k_x = \mathbb{1} \right]$$

• $\rho^\dagger = \rho$ • $\text{Tr}\{\rho'\} = \sum_k \text{Tr}\{k_x^\dagger k_x \rho\} = \text{Tr}\{\rho\}$ (EV von ρ)

• $\langle \psi | \rho' | \psi \rangle = \sum_k \langle \psi | k_x \rho k_x^\dagger | \psi \rangle = \sum_k |\langle \psi | k_x | \psi \rangle|^2 \rho_k \geq 0$ (EV von ρ)

$\rho = \sum_k \rho_k |u_k\rangle \langle u_k|$ (EV von ρ)

• Lindblad-GLE: $\dot{\rho} = -i[H, \rho] + \sum_k \left[L_k \rho L_k^\dagger - \frac{1}{2} L_k^\dagger L_k \rho - \frac{1}{2} \rho L_k^\dagger L_k \right]$

3.1.4. Entropie

Von-Neumann-Entropie

$$S_{\text{VN}}(\rho) = -\text{Tr}\{\rho \ln \rho\}$$

EV von ρ

$$\rho = \sum_k \rho_k |u_k\rangle \langle u_k|$$

$$\ln \rho = \sum_k \ln(\rho_k) |u_k\rangle \langle u_k|$$

$$S_{\text{VN}}(\rho) = \sum_k -\rho_k \ln \rho_k = S_{\text{Sh}}(\{\rho_k\})$$

$\rho \rightarrow \rho_D = \sum_{i,j} |i\rangle \langle j| \rho_{ij} \langle i| \langle j| = \sum_i \langle i | \rho | i \rangle |i\rangle \langle i|$ (diag. Anteil der DM)

z.B. $\rho = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \rightarrow \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Wie verhält sich $S_{\text{VN}}(\rho)$ zu $S_{\text{VN}}(\rho_D)$

• $D(\rho || \rho_D) = \text{Tr}\{\rho \ln \rho - \rho \ln \rho_D\} \geq 0$ (zwei gültige DM, Stupp)

• klar: $D(\rho || \rho) = 0$

$D(\rho || \rho_D) \neq D(\rho_D || \rho)$

$D(\rho || \rho_D) = -S_{\text{VN}}(\rho) - \text{Tr}\{\rho \ln \rho_D\} = -S_{\text{VN}}(\rho) - \text{Tr}\{\rho \sum_i \ln \rho_{ii} |i\rangle \langle i|\}$ (Diagonalelemente)

$= -S_{\text{VN}}(\rho) + S_{\text{VN}}(\rho_D) \geq 0$

$\rightarrow S_{\text{VN}}(\rho_D) \geq S_{\text{VN}}(\rho)$

$S\left(\frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\right) = 0$

$S\left(\frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right) = \ln 2$

3.1.5 Gibbs-Zustand

a.) Maximiere S unter NB: $\text{Tr}\{\rho\} = 1$

$\rho = \sum_k \rho_k |u_k\rangle \langle u_k| \rightarrow \rho_k = \frac{1}{N}$ (EV)

$\rho^* = \sum_k \frac{1}{N} |u_k\rangle \langle u_k| = \frac{1}{N} \cdot \mathbb{1}$ (EV)

$U \neq U^* = U \rightarrow$ gilt basis-unabhängig

b.) Fundare $\text{Tr}\{\rho\} = 1, \text{Tr}\{\rho \cdot H\} = U$

$\tilde{S} = S_W(\rho) + \lambda [\text{Tr}\{\rho\} - 1] + \beta [\text{Tr}\{\rho H\} - U] \rightarrow$ extensiv

$H = \sum_i E_i |\alpha\rangle\langle\alpha| \quad \langle\alpha|\rho|\alpha\rangle = p_{\alpha}$

\uparrow \uparrow
EV von H EV von H

$\tilde{S} = S_W(\rho) + \lambda [\sum_i p_{\alpha} - 1] + \beta [\sum_i p_{\alpha} \cdot E_i - U]$

\Rightarrow NB können nur von p_{α} in Energie-EB ab

$\rightarrow \alpha \neq \alpha' : \langle\alpha|\rho|\alpha'\rangle = 0$

$\rightarrow \rho^*$ ist diagonal in Energie-EB $p_{\alpha\alpha} = \frac{e^{-\beta E_{\alpha}}}{Z_c}$

$p_c = \frac{e^{-\beta H}}{\text{Tr}\{e^{-\beta H}\}}$

kanonische Gibbs-Zustand

$\langle A \rangle_c = \text{Tr}\{A \rho_c\}$

c.) $\text{Tr}\{\rho\} = 1, \text{Tr}\{\rho \cdot H\} = U, \text{Tr}\{\rho \cdot \hat{N}\} = N, \hat{N} = a^{\dagger}a$

falls $[\hat{H}, \hat{N}] = 0$

$p_{gc} = \frac{e^{-\beta(H - \mu \hat{N})}}{\text{Tr}\{e^{-\beta(H - \mu \hat{N})}\}}$ großk. Gibbs-Zustand

Druck von: $+ p = -\partial_b \ln Z_c = \frac{\text{Tr}\{H \cdot e^{-\beta H}\}}{\text{Tr}\{e^{-\beta H}\}}$

+ falls $H = H_0 + b \cdot H_1$ allg. $[\hat{H}_0, \hat{H}_1] \neq 0$

$\langle H_1 \rangle_c = -\frac{1}{b} \cdot \partial_b \ln Z_c = -\frac{1}{b} \frac{1}{Z_c} \text{Tr}\{\partial_b e^{-\beta(H_0 + b \cdot H_1)}\}$

$= -\frac{1}{b} \frac{1}{Z_c} \sum_{k=0}^{\infty} \text{Tr}\{\partial_b \frac{(-\beta)^k}{k!} (H_0 + b \cdot H_1)^k\} = -\frac{1}{b} \frac{1}{Z_c} \sum_{k=0}^{\infty} \text{Tr}\{\frac{(-\beta)^k}{k!} (H_0 + b \cdot H_1)^k H_1 \times (H_0 + b \cdot H_1)^{k-k-1}\}$

$= \text{Tr}\{H_1 \rho_c\} =$

-Trick geht nur für das 1. Moment von H_1

3.1.6. HO

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2 = \hbar \omega \left(a^\dagger a + \frac{1}{2} \right)$$

$$[a, a^\dagger] = 1$$

$$[\hat{x}, \hat{p}] = i\hbar$$

$$a^\dagger a |n\rangle = n |n\rangle$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a) \quad \hat{p} = i \sqrt{\frac{\hbar m \omega}{2}} (a^\dagger - a)$$

$$Z_c = \text{Tr} \{ e^{-\beta \hat{H}} \} = \sum_{k=0}^{\infty} \langle k | e^{-\beta \hbar \omega (a^\dagger a + 1/2)} | k \rangle$$

$$= \sum_{k=0}^{\infty} e^{-\beta \hbar \omega (k + 1/2)} = \frac{1}{e^{\beta \hbar \omega / 2} - e^{-\beta \hbar \omega}}$$

$$\rho_c = \frac{e^{-\beta \hbar \omega (a^\dagger a + 1/2)}}{Z_c} = \sum_{k=0}^{\infty} \frac{e^{-\beta \hbar \omega (k + 1/2)}}{Z_c} |k\rangle\langle k|$$

$$\langle x \rangle \propto \text{Tr} \{ (a + a^\dagger) \rho_c \}$$

$$a |k\rangle = \sqrt{k} |k-1\rangle$$

$$a^\dagger |k\rangle = \sqrt{k+1} |k+1\rangle$$

$$a |k\rangle\langle k| = \sqrt{k} |k-1\rangle\langle k|$$

$$\langle x \rangle = 0 = \langle p \rangle$$

$$\text{Tr} \{ P_k |k-1\rangle\langle k| \sqrt{k} + P_k |k+1\rangle\langle k| \sqrt{k+1} \}$$

$$\text{Tr} \{ |k-1\rangle\langle k| \} = \sum_n \langle n | |k-1\rangle\langle k| | n \rangle = \langle k | k-1 \rangle = 0$$

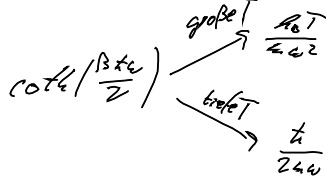
$$\langle x^2 \rangle = \frac{\hbar}{2m\omega} \text{Tr} \{ (a + a^\dagger)^2 \rho_c \}$$

$$= \frac{\hbar}{2m\omega} \text{Tr} \{ (a^2 + a^{\dagger 2} + a a^\dagger + a^\dagger a) \rho_c \}$$

$$\langle \frac{1}{2} m \omega^2 x^2 \rangle = \frac{\hbar \omega}{2}$$

$$= \frac{\hbar}{2m\omega} \sum_{k=0}^{\infty} \langle k | (a^\dagger a + a a^\dagger + 1) \rho_c \rangle$$

$$= \frac{\hbar}{2m\omega} \sum_{k=0}^{\infty} (2k+1) \frac{e^{-\beta \hbar \omega (k + 1/2)}}{Z_c} = \frac{\hbar}{2m\omega} \coth \left(\frac{\beta \hbar \omega}{2} \right)$$



and bei $T=0$ ist $\langle x^2 \rangle > 0$

$$\langle \frac{1}{2} m \omega^2 x^2 \rangle = \frac{\hbar \omega}{4}$$

= Hälfte der 0T-Energie

analoges $H = \frac{\hat{p}^2}{2m} + \left(\frac{1}{2} m \omega^2 \right) x^2$

$$\langle x^2 \rangle = -\frac{1}{\hbar} \frac{\partial}{\partial \left(\frac{1}{2} m \omega^2 \right)} \ln Z_c = -\frac{1}{m \omega^2} \frac{\partial}{\partial \omega} \ln Z_c$$

$$= -\frac{1}{\hbar} \frac{\partial}{\partial \omega} \ln Z_c$$