- Abgabe Übung → Di
- gemeint ist unendlich tiefer Pot.-topf

<u>Wdh</u>:
+ $\dot{\rho} = -\frac{i}{\hbar}[H, \rho] \rightsquigarrow \rho(t) = U(t)\,\rho_0\, U^\dagger(t)$

+ $S_{vN}(\rho) = -\mathrm{Tr}\{\rho \ln \rho\} = -\sum_\lambda \rho_\lambda \ln \rho_\lambda = S_{Sh}(\{\rho_\lambda\})$

  $\rho = \sum_\lambda \underbrace{\rho_\lambda}_{\text{EW von } \rho} |\underbrace{v_\lambda}_{\text{EV}}\rangle\langle v_\lambda|$ ist basis-unabhängig

+ $\underbrace{S_{vN}(\rho_D)}_{\text{ist basisabhängig}}$ $\qquad \rho_D = \sum_i |i\rangle\langle i|\rho|i\rangle\langle i|$

$\Rightarrow S_{vN}(\rho_D) \geq S_{vN}(\rho)$

$\Rightarrow$ a.) $\mathrm{Tr}\{\rho\} = 1 \rightsquigarrow \rho^* = \frac{1}{N}\cdot\mathbb{1}$ maximiert $S_{vN}(\rho^*)$

b.) $\mathrm{Tr}\{\rho\} = 1 \quad \mathrm{Tr}\{\hat{H}\rho\} = E \rightsquigarrow \rho^* = \frac{e^{-\beta\hat{H}}}{\mathrm{Tr}\{e^{-\beta\hat{H}}\}} \rightsquigarrow \boxed{Z_c = \mathrm{Tr}\{e^{-\beta\hat{H}}\}}$

c.) " $\quad$ " $\quad \mathrm{Tr}\{\hat{N}\rho\} = N \rightsquigarrow \rho^* = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}\{\text{"}\}}$

$\boxed{Z_{gc} = \mathrm{Tr}\{e^{-\beta(\hat{H}-\mu\hat{N})}\}}$

Messprozess: $\hat{O} = \sum_n \lambda_n |v_n\rangle\langle v_n|$

projektive Messung

+ $\hat{H} = \hat{H}_0 + b\cdot\hat{H}_1 \qquad [\hat{H}_0, \hat{H}_1] \neq 0$

  $\rightsquigarrow \langle H_1\rangle = -\frac{1}{\beta}\frac{\partial}{\partial b}\ln \mathrm{Tr}\{e^{-\beta\hat{H}}\}$

+ Bsp: HO

  $\langle\hat{x}\rangle_c = \langle\hat{p}\rangle_c = 0$

  $\langle \frac{1}{2} m\omega^2 \hat{x}^2\rangle = \frac{\hbar\omega}{4}\coth\left(\frac{\beta\hbar\omega}{2}\right) \xrightarrow{\beta\hbar\omega \gg 1} \frac{\hbar\omega}{4}$ halbe Nullpunktsenergie

  $\xrightarrow{\beta\hbar\omega \ll 1} \frac{1}{2}k_B T$

  $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$

$\langle \hat{x}^3 \rangle \ldots \langle \hat{x}^4 \rangle$

3.2. Quantengase

3.2.1. Einschub: Leiteroperatoren

HO: $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{q}^2 = \hbar\omega \left(\underbrace{a^\dagger a}_{\hat{N}} + 1/2 \right)$

$[a, a^\dagger] = 1$ Fock-Zustände

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

$a |n\rangle = \sqrt{n}\, |n-1\rangle$

formale Eigenschaften: $\boxed{\begin{array}{l} [a^\dagger a, a] = -a \\ [\underbrace{a^\dagger a}_{\hat{N}}, a^\dagger] = +a^\dagger \end{array}}$

$\langle n | a^\dagger a | n \rangle = n \qquad n \in \{0, 1, 2, \ldots\}$

$\frac{d}{dt} e^{+i\omega t a^\dagger a} = i\omega a^\dagger a\, e^{+i\omega t a^\dagger a} = e^{+i\omega t a^\dagger a}\, i\omega a^\dagger a$

$\rightsquigarrow e^{+i\omega t a^\dagger a}\, a\, e^{-i\omega t a^\dagger a} = \hat{a}(t)$

$\frac{d}{dt} \hat{a}(t) = e^{+i\omega t a^\dagger a} [i\omega a^\dagger a, a]\, e^{-i\omega t a^\dagger a} = -i\omega\, \hat{a}(t) \rightsquigarrow \hat{a}(t) = e^{-i\omega t} a$

$\hat{a}^\dagger(t) = e^{+i\omega t} a^\dagger$

Möglichkeit a)	Möglichkeit b)
$\to [a_b, a_b^\dagger] = +1$	$\{a_f, a_f^\dagger\} = 1 = a_f a_f^\dagger + a_f^\dagger a_f$
$\|n\rangle : n \in \{0, 1, 2, \ldots\}$	$\{a_f, a_f\} = 0$, $\{a_f^\dagger, a_f^\dagger\} = 0$ $\Big\}$ $a_f^2 = (a_f^\dagger)^2 = 0$
$a_b^\dagger a_b a_b - a_b a_b^\dagger a_b \overset{!}{=} -a_b$	$\rightsquigarrow \|n\rangle : n \in \{0, 1\}$
	$a_f^\dagger \underbrace{a_f a_f}_{=0} - a_f \underbrace{a_f^\dagger a_f}_{1 - a_f a_f^\dagger} = -a_f$

bisher nur eine Mode jetzt: viele $1 \le k \le K$ $\hat{H} = \sum_{k=1}^{K} \hat{a}_k^\dagger \hat{a}_k$

$[\hat{N}, \hat{a}_k] = -\hat{a}_k \qquad [\hat{N}, \hat{a}_k^\dagger] = +a_k^\dagger$

$a_k^\dagger a_k |n_1, \ldots, n_K\rangle = n_k |n_1, \ldots, n_K\rangle$

N_{cut} ≙ Anzahl Zust. für eine Mode $\to N_{cut} \to \infty$, $N_{cut} = 2$

$(N_{cut})^K$

$1 \le k \le K$

bosonisch

$[a_k, a_q^\dagger] = \delta_{kq} \qquad n_k \in \{0, 1, 2, \ldots\}$

$[a_k, a_q] = 0$

$a_k |n_1 \ldots n_{k-1} n_k n_{k+1} \ldots n_K\rangle = \sqrt{n_k}\, |n_1 \ldots (n_k - 1), \ldots, n_K\rangle$

fermionisch

$\{a_k, a_q^\dagger\} = \delta_{kq} \qquad n_k \in \{0, 1\}$

$\{a_k, a_q\} = 0 \Rightarrow a_k^2 = 0$

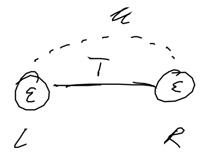
$a_k |n_1 \ldots n_{k-1}, 1, n_{k+1}, \ldots, n_K\rangle = \pm |n_1 \ldots 0 \ldots n_K\rangle$

$|0 \ldots 0\rangle \qquad a_1^\dagger |0 \ldots 0\rangle = |1\, 0 \ldots 0\rangle$

3.2.2. Doppelquantenpunkt

$\{d_i, d_j^\dagger\} = \delta_{ij} \qquad \{d_i, d_j\} = 0$

fermion. Operatoren



$$\hat{H} = \varepsilon\left(d_1^\dagger d_1 + d_2^\dagger d_2\right) + \underbrace{T}_{\text{Tunnel-Kopl.}}\left(d_1^\dagger d_2 + d_2^\dagger d_1\right) + \underbrace{U}_{\text{Coulomb-Abstoßung}} d_1^\dagger d_1 d_2^\dagger d_2$$

$|n_1, n_2\rangle$

④ $|0,0\rangle$

③ $|0,1\rangle = -d_2^\dagger |0,0\rangle$

② $|1,0\rangle = d_1^\dagger |0,0\rangle$

① $|1,1\rangle = d_2^\dagger d_1^\dagger |0,0\rangle$

$\langle 1,1|\hat{H}|1,1\rangle$

$$\Rightarrow \hat{H} = \begin{pmatrix} 2\varepsilon + U & 0 & 0 & 0 \\ 0 & \varepsilon & -T & 0 \\ 0 & -T & \varepsilon & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\hat{N} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

a) kanonisch

$$\varrho_c = \frac{e^{-\beta \hat{H}}}{\mathrm{Tr}\{e^{-\beta \hat{H}}\}}$$

falls $N = \text{const}$

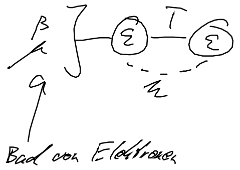
$\varrho_c^{(0)} = |0,0\rangle\langle 0,0|$

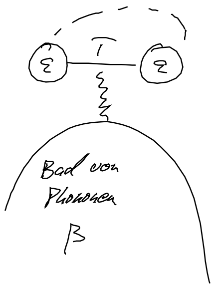
$\varrho_c^{(2)} = |1,1\rangle\langle 1,1|$

$$\varrho_c^{(1)} = \frac{\exp\left[-\beta \begin{pmatrix} \varepsilon & -T \\ -T & \varepsilon \end{pmatrix}\right]}{\mathrm{Tr}\{\dots\}}$$

b.) großkanonisch

$$\varrho_{gc} = \frac{e^{-\beta(\hat{H} - \mu \hat{N})}}{\mathrm{Tr}\{\,\text{''}\,\}}$$





$\langle N \rangle = \mathrm{Tr}\{\hat{N} \varrho_{gc}\}$

3.2.3. Nichtwechselwirkende Quantengase (ideale Quantengase)

$$\hat{N} = \sum_k \underbrace{a_k^\dagger a_k}_{\text{Bosonen oder Fermionen}} \qquad \hat{H} = \sum_k \underbrace{\varepsilon_k}_{\text{ET-Energie}} a_k^\dagger a_k \quad \text{nicht-ww}$$

$$\hat{H}|n_1 \dots n_N\rangle = \underbrace{\sum_k \varepsilon_k \cdot n_k}_{\varepsilon_n} |n_1 \dots n_N\rangle = \varepsilon_{\underline{n}} |\underline{n}\rangle$$

$$k \neq q: \left[a_k^\dagger a_k, a_q^\dagger a_q\right] = a_k^\dagger a_k a_q^\dagger a_q - a_q^\dagger a_q a_k^\dagger a_k = 0$$

$$e^{A+B} \overset{[A,B]=0}{=} e^{A} e^{B}$$

$$\rho_c = \frac{e^{-\beta \hat{H}}}{\mathrm{Tr}\{\cdot\}} = \frac{\prod_k e^{-\beta \epsilon_k a_k^\dagger a_k}}{\sum_{n_1}\dots\sum_{n_K} \langle n_1 \dots n_K | \prod_k e^{-\beta \epsilon_k a_k^\dagger a_k} | n_1 \dots n_K \rangle} = \prod_k \frac{e^{-\beta \epsilon_k a_k^\dagger a_k}}{\sum_{n_k} \langle n_k | e^{-\beta \epsilon_k a_k^\dagger a_k} | n_k \rangle}$$

$$= \prod_k \rho_c^{(k)}$$

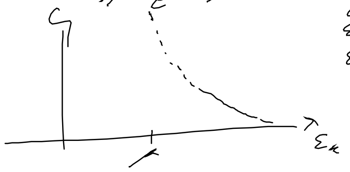
ρ_{gc} geht analog

a.) bosonisch

$$Z_{gc}^{(k)} = \sum_{n=0}^{\infty} e^{-\beta(\epsilon_k - \mu)\cdot n} \overset{\text{falls } \epsilon_k - \mu > 0}{=} \frac{1}{1 - e^{-\beta(\epsilon_k - \mu)}} \quad \rightsquigarrow \mu < \epsilon_k \;\; \forall k$$

$$\boxed{\langle n_k \rangle = \langle a_k^\dagger a_k \rangle = \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1}}$$

Bose-Einstein-Verteilung



chem. Pot. ist bei Bosonen eingeschränkt

$\epsilon_{min} = 0$

$\epsilon_k \geq 0 \rightsquigarrow \mu \leq 0$

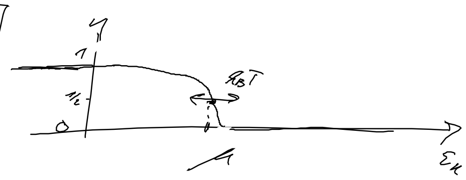
b.) fermionisch

$$Z_{gc}^{(k)} = \sum_{n=0}^{1} e^{-\beta(\epsilon_k - \mu)\cdot n} = 1 + e^{-\beta(\epsilon_k - \mu)}$$

$$\boxed{\langle n_k \rangle = \langle a_k^\dagger a_k \rangle = \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1}}$$

Fermi-Dirac-Verteilung

chem. Pot ist nicht eingeschränkt



für $\beta(\epsilon_k - \mu) \gg 1 \rightsquigarrow \langle n_k \rangle \approx e^{-\beta(\epsilon_k - \mu)}$