Wdh

Vektorisierung $\quad \rho = \sum_{ij} \rho_{ij} |i\rangle\langle j| \quad \Longleftrightarrow \quad vec(\rho) = \sum_{ij} \rho_{ij} |i\rangle \otimes |j\rangle$

$$A \otimes B = \begin{pmatrix} A_{11}\cdot B & A_{12}\cdot B & \cdots & A_{1N_A}\cdot B \\ A_{21}\cdot B & & & \vdots \\ \vdots & & & \vdots \\ A_{N_A 1}\cdot B & \ldots & & A_{N_A N_A}\cdot B \end{pmatrix}$$

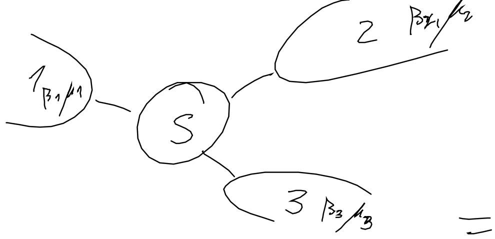
$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1\cdot\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad \rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} \Longleftrightarrow vec(\rho) = \begin{pmatrix} \rho_{00} \\ \rho_{01} \\ \rho_{10} \\ \rho_{11} \end{pmatrix}$$

$$vec(A\rho B) = \left(A \otimes B^T\right) vec(\rho) \qquad Tr\{\hat{O}\} = \left[vec(\mathbb{1})\right]^T \cdot vec(\hat{O})$$

Notation hier: $vec(\rho)$ weglassen

Superoperatoren kalligrafisch

• Nichtgleichgewicht



$$\bar{\rho}_B = \bigotimes_\nu \frac{e^{-\beta_\nu\left[H_B^{(\nu)} - \mu_\nu N_B^{(\nu)}\right]}}{Z_B^{(\nu)}}$$

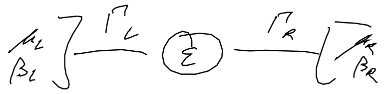
Dissipator für das Reservoir ν

$$\Rightarrow \mathcal{L} = \mathcal{L}^{(0)} + \sum_\nu \mathcal{L}^{(\nu)}$$

$$\mathcal{L}^{(0)}\rho \hat{=} -i[H,\rho]$$

Super-Operator

Bsp:



$$\sum_\nu \Gamma_\nu \begin{pmatrix} -f_\nu & 1-f_\nu \\ f_\nu & -(1-f_\nu) \end{pmatrix} = \mathcal{L}_{pop} \qquad \begin{matrix} |0\rangle \\ |1\rangle \end{matrix}$$

$$\mathcal{L} = \left(\sum_\nu \mathcal{L}^{(\nu)}\right) + \mathcal{L}^{(0)} \rightsquigarrow \frac{d}{dt}\langle E\rangle = \sum_\nu \underbrace{Tr\{H_S(\mathcal{L}^{(\nu)}\rho(t))\}}_{I_E^{(\nu)}(t)}$$

$$I_N^{(\nu)} = Tr\{N_S(\mathcal{L}^{(\nu)}\rho(t))\}$$

. . .

Phänomenologisch

2.3. Nichtgleichgewichts-TD

• Startpunkt $\dot\rho = -i[H_S(t), \rho] + \sum_\nu \mathcal{L}^{(\nu)}_{(t)} \rho$ (sehr langsames Treiben)

• Energiebilanz: $\dot E = \frac{d}{dt} \mathrm{Tr}\{H_S(t) \rho(t)\}$

$dU = dQ + \mu dN$

$\frac{dQ}{dt} = \frac{dU}{dt} - \mu \frac{dN}{dt}$

$$= \mathrm{Tr}\{\dot H_S \rho\} + \sum_\nu \mathrm{Tr}\{H_S (\mathcal{L}^{(\nu)}_{(t)} \rho)\}$$

$$= \underbrace{\mathrm{Tr}\{\dot H_S \rho\}}_{\text{mech. Arbeitsrate}} + \underbrace{\sum_\nu \mu_\nu \mathrm{Tr}\{N_S (\mathcal{L}^{(\nu)}(t) \rho)\}}_{\text{chem. Arbeitsrate}} + \sum_\nu \underbrace{\mathrm{Tr}\{(H_S - \mu_\nu N_S)(\mathcal{L}^{(\nu)}_{(t)} \rho)\}}_{\dot Q^{(\nu)}}$$

Wärmestrom aus Reservoir ν

1. Hauptsatz

⇝ weitere Annahme $\mathcal{L}^{(\nu)}_{(t)} \underbrace{\frac{e^{-\beta_\nu [H_S(t) - \mu_\nu N_S]}}{Z_S}}_{\bar\rho^{(\nu)}(t)} = 0$

$$\ln \bar\rho^{(\nu)}(t) = -\beta_\nu [H_S(t) - \mu_\nu N_S] - (\ln Z_S) \mathbf{1}$$

$$\dot S_i = \underbrace{\dot S}_{\text{System}} + \sum_\nu \underbrace{\dot S^{(\nu)}_{res}}_{\text{Reservoir}}$$

$$= -\frac{d}{dt} \mathrm{Tr}\{\rho \ln \rho\} - \sum_\nu \beta_\nu \dot Q^{(\nu)}$$

$\frac{d}{dt} \mathrm{Tr}\{\rho \ln \rho\} = \mathrm{Tr}\{\dot\rho \ln \rho\} + 0$

$$= \sum_\nu \underbrace{-\mathrm{Tr}\{(\mathcal{L}^{(\nu)}(t) \rho(t)) [\ln \rho(t) - \ln \bar\rho^{(\nu)}(t)]\}}_{\geq 0}$$

$\mathrm{Tr}\{\mathcal{L}^{(\nu)} \rho\} = 0$

Spohn'sche Ungleichung

$$\boxed{\dot S_i = \dot S - \sum_\nu \underbrace{\beta_\nu \dot Q^{(\nu)}}_{(-\dot S^{(\nu)}_{res})} \geq 0}$$

irreversible Entropieproduktionsrate

2. Hauptsatz

• $\dot S < 0$ ist möglich

2.4. Langzeitlimes

$$\dot S_i \longrightarrow -\sum_\nu \beta_\nu \bar{\dot Q}^{(\nu)} = -\sum_\nu \beta_\nu [\bar I_E^{(\nu)} - \mu_\nu \bar I_M^{(\nu)}] \geq 0$$

z.B.: 2-Terminal

kein Treiben $H_S(t) = H_S$

$\bar I_E^{(L)} + \bar I_E^{(R)} = 0$

$\bar I_M^{(L)} + \bar I_M^{(R)} = 0$

$$\left.\begin{aligned} \bar I_E &= \bar I_E^{(L)} = -\bar I_E^{(R)} \\ \bar I_M &= \bar I_M^{(L)} = -\bar I_M^{(R)} \end{aligned}\right\} \text{Ströme von links nach rechts}$$

$$\dot{S}_i = (\beta_R-\beta_L)\bar{I}_E + (\mu_L\beta_L - \mu_R\beta_R)\bar{I}_M \geq 0$$

a.) $\beta_L=\beta_R=\beta \rightsquigarrow (\mu_L-\mu_R)\cdot\bar{I}_M \geq 0$ Strom fließt von hohen zu niedrigen chem. Potential

b.) $\mu_L=\mu_R=\mu \rightsquigarrow (\beta_R-\beta_L)\underbrace{(\bar{I}_E-\mu\bar{I}_M)}_{\dot{\bar{Q}}_{L\to R}} \geq 0$ Wärme fließt von selbst von heiß nach kalt

c.) $\mu_L<\mu_R \quad \beta_L<\beta_R \quad (T_L>T_R)$

$$\eta = \frac{-\bar{I}_M(\mu_L-\mu_R)}{\bar{I}_E-\mu_L\cdot\bar{I}_M} = \frac{-(\beta_R-\beta_L)(\mu_L-\mu_R)\bar{I}_M}{(\beta_R-\beta_L)\bar{I}_E-(\beta_R-\beta_L)\mu_L\cdot\bar{I}_M+(\mu_L\beta_L-\mu_R\beta_R)\bar{I}_M-(\mu_L\beta_L-\mu_R\beta_R)\bar{I}_M}$$

$$\leq \frac{-(\beta_R-\beta_L)(\mu_L-\mu_R)\cancel{\bar{I}_M}}{-(\mu_L\beta_L-\mu_R\beta_R)\cancel{\bar{I}_M}-(\beta_R-\beta_L)\mu_L\cancel{\bar{I}_M}} = 1-\frac{\beta_L}{\beta_R} = 1-\frac{T_R}{T_L} = 1-\frac{T_{cold}}{T_{hot}} = \eta_{Carnot}$$

Effizienz für die Umwandlung von Wärme in chem. Arbeit [≙ beim SET elektr. Leistung]

analog $\quad COP_{cooling} := \frac{-(\bar{I}_E-\mu_R\bar{I}_M)}{(\mu_L-\mu_R)\cdot\bar{I}_M} = \ldots \leq \frac{T_{cold}}{T_{hot}-T_{cold}}$

2.5. Beispiel: SET

$$Z = \begin{pmatrix} -\Gamma_L\cdot f_L-\Gamma_R\cdot f_R & +\Gamma_L(1-f_L)+\Gamma_R(1-f_R) \\ +\Gamma_L f_L+\Gamma_R\cdot f_R & -\Gamma_L(1-f_L)-\Gamma_R(1-f_R) \end{pmatrix}$$

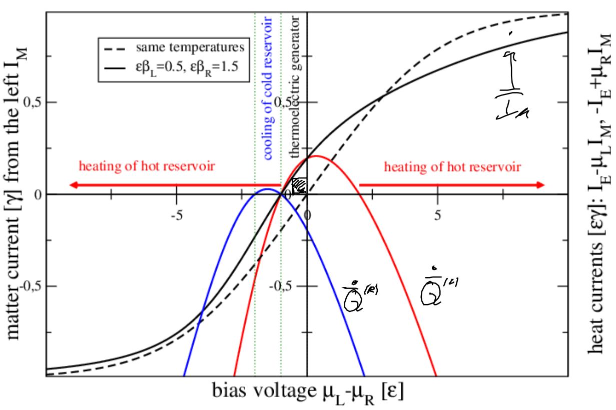
$\Gamma_\nu = \Gamma_\nu(\varepsilon) \qquad f_\nu = \frac{1}{e^{\beta_\nu(\varepsilon-\mu_\nu)}+1}$

$$\bar{I}_E = \bar{I}_E^{(L)} = \frac{\Gamma_L\cdot\Gamma_R}{\Gamma_L+\Gamma_R}\cdot\varepsilon(f_L-f_R) = \varepsilon\cdot\bar{I}_M$$

$P = -(\mu_L-\mu_R)\cdot\bar{I}_M$

$\dot{Q}^{(L)} = \bar{I}_E-\mu_L\bar{I}_M$

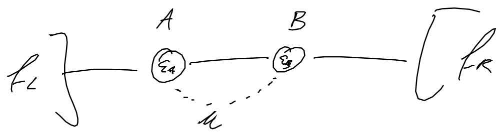
$\dot{Q}^{(R)} := -(\bar{I}_E-\mu_R\bar{I}_M)$



$\beta_R > \beta_L \quad (T_R < T_L)$

$\mu_L = +\frac{V}{2} \quad \mu_R = -\frac{V}{2}$

2.6 Beispiel DQD



$$H_S = \varepsilon_A d_A^\dagger d_A + \varepsilon_B d_B^\dagger d_B + T\left(d_A d_B^\dagger + d_B d_A^\dagger\right) + U d_A^\dagger d_A d_B^\dagger d_B$$

$$H_B = \sum_k \varepsilon_{kL} d_{kL}^\dagger d_{kL} + \sum_k \varepsilon_{kR} d_{kR}^\dagger d_{kR}$$

$$H_I = \sum_k \left(t_{kL} d_A c_{kL}^\dagger + h.c.\right) + \sum_k \left(t_{kR} d_B c_{kR}^\dagger + h.c.\right)$$

$|0\rangle = |00\rangle$
$|01\rangle$
$|10\rangle$
$|2\rangle = |11\rangle$

$$H_S = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \varepsilon_B & T & 0 \\ 0 & T & \varepsilon_A & 0 \\ 0 & 0 & 0 & \varepsilon_A + \varepsilon_B + U \end{pmatrix}$$

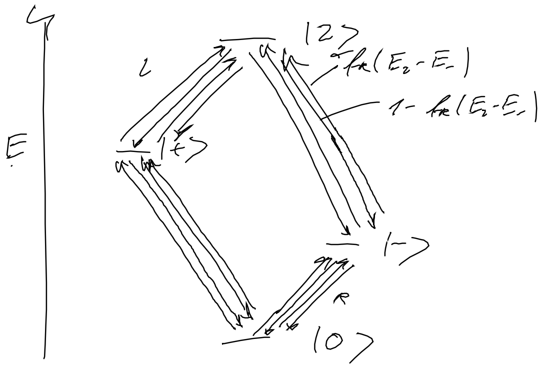
$E_0 = 0$ $\quad |0\rangle$

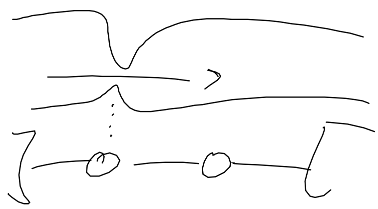
$E_\pm = \frac{\varepsilon_A + \varepsilon_B}{2} \pm \sqrt{\left(\frac{\varepsilon_B - \varepsilon_A}{2}\right)^2 + T^2}$ $\quad |\pm\rangle$

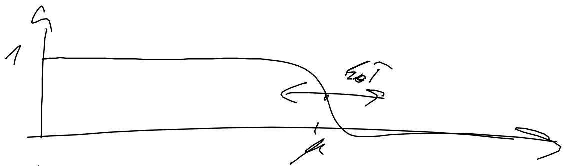
$E_2 = \varepsilon_A + \varepsilon_B + U$ $\quad |2\rangle$

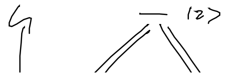
Ratengleichung $\quad \dot{\rho}_{aa} = \sum_b \gamma_{ab,ab}\, \rho_{bb} - \sum_b \gamma_{ba,ba} \cdot \rho_{aa}$

$$\gamma_{ab,ab} = \sum_{\alpha\beta} \gamma_{\alpha\beta}(E_b - E_a) \cdot \langle a|A_\beta|b\rangle \langle a|A_\alpha^\dagger|b\rangle^* \qquad \text{CG: } \tau \to \infty$$









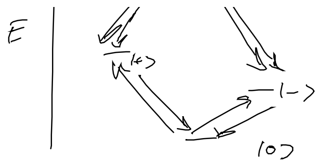
Vereinfachung: ° Coulomb-Blockade

$f_\nu(x + U) = 0$

° große Spannung $f_L \gg f_R$

$f_L(E_\pm - E_0) \to 1$

$f_R(E_\pm - E_0) \to 0$



$\beta_L = \beta_R = \beta$

$\mu_L = +\frac{V}{2}$

$\mu_R = -\frac{V}{2}$

tiefe Temperaturen