

WdK

Vektorenraum $\rho = \sum_{ij} \rho_{ij} |i\rangle\langle j| \iff \text{vec}(\rho) = \sum_{ij} \rho_{ij} |i\rangle \otimes |j\rangle$

$$A \otimes B = \begin{pmatrix} A_{11} \cdot B & A_{12} \cdot B & \dots & A_{1n} \cdot B \\ A_{21} \cdot B & & & \\ \vdots & & & \\ A_{m1} \cdot B & \dots & \dots & A_{mn} \cdot B \end{pmatrix}$$

$$\begin{pmatrix} 1 & \\ & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & 0 \end{pmatrix} = \begin{pmatrix} 1 \cdot \begin{pmatrix} 1 & \\ & 0 \end{pmatrix} & \\ & 0 \cdot \begin{pmatrix} 1 & \\ & 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & 0 \end{pmatrix}$$

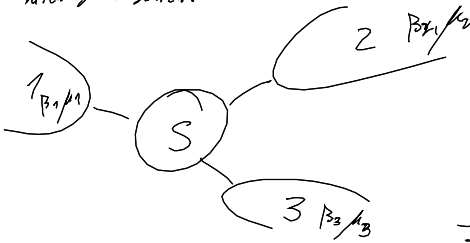
$$\rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} \iff \text{vec}(\rho) = \begin{pmatrix} \rho_{00} \\ \rho_{01} \\ \rho_{10} \\ \rho_{11} \end{pmatrix}$$

$$\text{vec}(A \rho B) = (A \otimes B^T) \text{vec}(\rho)$$

$$\text{Tr}\{\hat{O}\} = [\text{vec}(\hat{O})]^T \cdot \text{vec}(\hat{O})$$

Notation hier: $\text{vec}(\rho)$ vergessen
Superoperatoren kolligiert

o Nichtgleichgewicht



$$\bar{\rho}_B = \frac{e^{-\beta \nu [\mathcal{H}_S^{(M)} - \mu N_B^{(M)}]}}{Z_B^{(M)}}$$

Dissipator für das Reservoir

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

$$\sum_{\nu} Z^{(\nu)} \approx -: [\mathcal{H}, \rho]$$

Super-Operator

Bsp: $\frac{\mu_L}{\beta_L} \left[\frac{\Gamma_L}{\Sigma} \right] \xrightarrow{\Gamma_R} \left[\frac{\Gamma_R}{\beta_R} \right]$

$$\sum_{\nu} \Gamma_{\nu} \begin{pmatrix} -\nu & 1-\nu \\ \nu & -(1-\nu) \end{pmatrix} = \sum_{\nu} \rho_{\nu} \begin{matrix} |0\rangle \\ |1\rangle \end{matrix}$$

$$Z = \left(\sum_{\nu} Z^{(\nu)} \right) + Z^{(0)} \rightarrow \frac{d}{dt} \langle E \rangle = \sum_{\nu} \text{Tr} \left\{ \mathcal{H}_S \left(\sum_{\nu} \Gamma_{\nu} \rho_{\nu} \right) \right\}$$

$$\Gamma_{\nu}^{(M)} = \text{Tr} \left\{ \mathcal{H}_S \left(\sum_{\nu} \Gamma_{\nu} \rho_{\nu} \right) \right\}$$

2.3. Nichtgleichgewichts-TD phänomenologisch

• Startpunkt $\dot{\rho} = -i[H_S(t), \rho] + \sum_\nu \mathcal{L}^{(\nu)} \rho$ (siehe langsame Treiber)

• Energiebilanz: $\dot{E} = \frac{d}{dt} \text{Tr}\{H_S(t) \rho(t)\}$
 $= \text{Tr}\{\dot{H}_S \rho\} + \sum_\nu \text{Tr}\{H_S (\mathcal{L}^{(\nu)} \rho)\}$
 $= \underbrace{\text{Tr}\{\dot{H}_S \rho\}}_{\text{rech. Arbeitsrate}} + \sum_\nu \underbrace{\text{Tr}\{H_S (\mathcal{L}^{(\nu)} \rho)\}}_{\text{chem. Arbeitsrate}} + \sum_\nu \underbrace{\text{Tr}\{(H_S - \mu H_S) (\mathcal{L}^{(\nu)} \rho)\}}_{\dot{Q}^{(\nu)}}$

$dH = dQ + \mu dN$
 $\frac{dQ}{dt} = \frac{dH}{dt} - \mu \frac{dN}{dt}$
 Wärmestrom aus Reservoir ν

1. Hauptsatz

→ stationäre Annahme $\sum_\nu \frac{e^{-\beta_V (H_S + \mu_V N_S)}}{Z_S} = 0$
 $\bar{\rho}^{(M)}(t)$

$\ln \bar{\rho}^{(M)}(t) = -\beta_V [H_S(t) + \mu_V N_S] - (\ln Z_S) \frac{1}{\mathcal{L}}$

$\dot{S}_i = \dot{S} + \sum_\nu \dot{S}_{res}^{(\nu)}$
 $= -\frac{d}{dt} \text{Tr}\{\rho \ln \rho\} - \sum_\nu \beta_V \dot{Q}^{(\nu)}$
 $= \sum_\nu \underbrace{\text{Tr}\{(\mathcal{L}^{(\nu)} \rho) [\ln \rho(t) - \ln \bar{\rho}^{(M)}(t)]\}}_{\geq 0 \text{ Spaltweise Ungleichung}} \quad \text{Tr}\{Z^{(M)} \rho\} = 0$

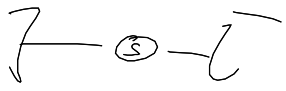
$\dot{S}_i = \dot{S} - \sum_\nu \beta_V \dot{Q}^{(\nu)} \geq 0$
 irreversible Entropieproduktionsrate $(-\dot{S}_{res}^{(M)})$
 2. Hauptsatz

$\dot{S} < 0$ ist möglich

2.4. Langzeitlimit

$\dot{S}_i \rightarrow -\sum_\nu \beta_V \dot{Q}^{(\nu)} = -\sum_\nu \beta_V [\overline{I}_E^{(\nu)} - \mu_V \overline{I}_N^{(\nu)}] \geq 0$

z.B.: Z-Terminal



kein Treiber $H_S(t) = H_S$
 $\overline{I}_E^{(L)} + \overline{I}_E^{(R)} = 0$
 $\overline{I}_N^{(L)} + \overline{I}_N^{(R)} = 0$

$\overline{I}_E = \overline{I}_E^{(L)} = -\overline{I}_E^{(R)}$
 $\overline{I}_N = \overline{I}_N^{(L)} = -\overline{I}_N^{(R)}$
 } Ströme von links nach rechts

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

a) $\beta_L = \beta_R = \beta \rightarrow (\mu_L - \mu_R) \cdot \bar{I}_A \geq 0$ Strom fließt von links zu rechts in über. Potential

b) $\mu_L = \mu_R = \mu \rightarrow (\beta_R - \beta_L) (\bar{I}_E - \bar{I}_A) \geq 0$
 $\underbrace{\hspace{10em}}_{\dot{Q}_{L \rightarrow R}}$ Wärme fließt von selbst von heiß nach kalt

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

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

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

Effizienz für die Umwandlung von Wärme in elektr. Arbeit (z.B. von SET abh. Lastung)

analog $COP_{\text{cooling}} = \frac{-(\bar{I}_E - \mu_L \bar{I}_A)}{(\mu_L - \mu_R) \cdot \bar{I}_A} = \dots \leq \frac{T_{\text{cold}}}{T_{\text{hot}} - T_{\text{cold}}}$

2.5. Resonant: SET

$$Z = \begin{vmatrix} -\Gamma_L \cdot k_L - \Gamma_R \cdot k_R & +\Gamma_L (1-k_L) + \Gamma_R (1-k_R) \\ +\Gamma_L k_L + \Gamma_R k_R & -\Gamma_L (1-k_L) - \Gamma_R (1-k_R) \end{vmatrix}$$

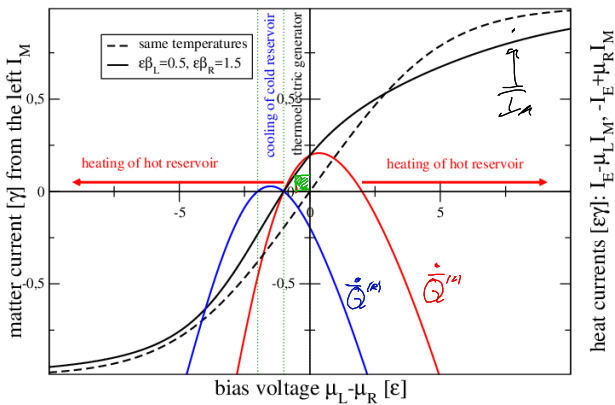
$$\Gamma_L = \Gamma_L(\varepsilon) \quad k_L = \frac{1}{e^{R_L(\varepsilon - \mu)} + 1} \quad \bar{I}_E = \bar{I}_E^{(L)} = \frac{\Gamma_L \cdot \Gamma_R}{\Gamma_L + \Gamma_R} \cdot \varepsilon (k_L - k_R)$$

$$= \varepsilon \cdot \bar{I}_A$$

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

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

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

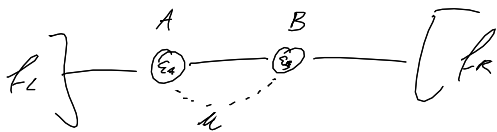


heat currents [εγ]: $\bar{I}_E - \mu_L \bar{I}_A$, $-\bar{I}_E + \mu_R \bar{I}_A$

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

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

Z. G. Beispiel DQD



$$H_S = \epsilon_A d_A^\dagger d_A + \epsilon_B d_B^\dagger d_B + T (d_A d_B^\dagger + d_B d_A^\dagger) + U d_A^\dagger d_A d_B^\dagger d_B$$

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

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

$|0\rangle = |00\rangle$
 $|1\rangle = |11\rangle$
 $|2\rangle = |11\rangle$

$$H_S = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \epsilon_B & T & 0 \\ 0 & T & \epsilon_A & 0 \\ 0 & 0 & 0 & \epsilon_A + \epsilon_B + U \end{pmatrix}$$

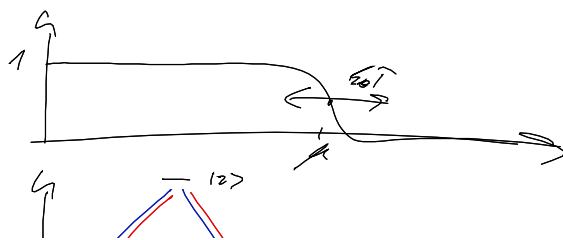
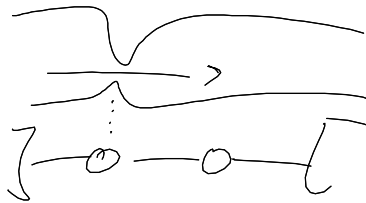
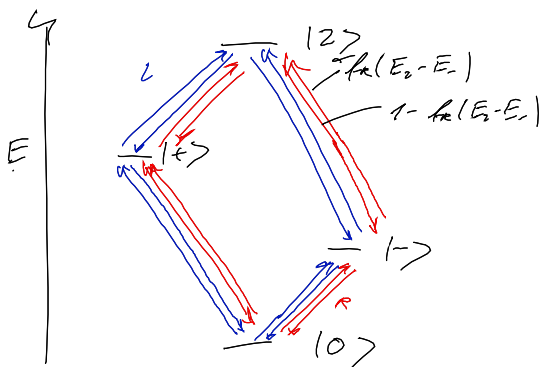
$$E_0 = 0 \quad |0\rangle$$

$$E_{\pm} = \frac{\epsilon_A + \epsilon_B}{2} \pm \sqrt{\left(\frac{\epsilon_A - \epsilon_B}{2}\right)^2 + T^2} \quad |1\rangle$$

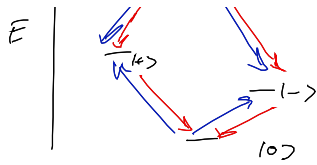
$$E_2 = \epsilon_A + \epsilon_B + U \quad |2\rangle$$

Ratengleichung $\dot{\rho}_{\alpha\beta} = \sum_{\gamma} \gamma_{\alpha\gamma\beta} \rho_{\gamma\beta} - \sum_{\gamma} \gamma_{\gamma\alpha\beta} \rho_{\alpha\gamma}$

$$\gamma_{\alpha\beta\gamma} = \sum_{\alpha', \beta'} \gamma_{\alpha\alpha'} (E_{\beta} - E_{\alpha'}) \cdot \langle \alpha | A_{\beta} | \alpha' \rangle \langle \alpha' | A_{\beta}^\dagger | \beta \rangle \quad CG: \tau \rightarrow \infty$$



Veranschaulichung : • Coulomb-Blockade
 $f_L(x+a) = 0$
 • große Spannung $\mu_L \gg \mu_R$
 $f_L(E_S - E_0) \rightarrow 1$
 $f_R(E_0 - E_1) \rightarrow 0$



$\beta_L = \beta_R = \beta$
 $\mu_L = \mu + \frac{eV}{2}$
 $\mu_R = \mu - \frac{eV}{2}$
 tiefe Temperaturen

