Wdh

- benchmark mit exakt lösbaren Modellen

i) spin-boson: pure dephasing

$$H = \underbrace{\frac{\omega}{2}\sigma^z}_{H_S} + \underbrace{\sigma^z}_{A} \otimes \underbrace{\sum_k \left(h_k b_k + h_k^* b_k^\dagger\right)}_{B} + \underbrace{\sum_k \omega_k b_k^\dagger b_k}_{H_B}$$

$\Rightarrow$ BMS-Mastergleichung
$$\frac{d}{dt}\begin{pmatrix}\rho_{00}\\ \rho_{11}\\ \rho_{01}\\ \rho_{10}\end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & \eta & 0\\ 0 & 0 & 0 & \eta^* \end{pmatrix}\begin{pmatrix}\rho_{00}\\ \rho_{11}\\ \rho_{01}\\ \rho_{10}\end{pmatrix}$$

$Re(\eta) \leq 0$ "Dekohärenz"

$$\rho_{01}(t) = e^{\eta \cdot t}\rho_{01}(0)$$

ii) SRL $\quad f(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}+1}$ — (ϵ)

$$H = \epsilon d^\dagger d + \left(d^\dagger \sum_k t_k c_k + h.c.\right) + \sum_k \epsilon_k c_k^\dagger c_k$$
quadratisch in d, c_k

$\rightsquigarrow$ exakt lösbar über Heisenberg-BWGL

BMS-MG

$$\frac{d}{dt}\begin{pmatrix}\rho_{00}\\ \rho_{11}\end{pmatrix} = \underbrace{\Gamma(\epsilon)\begin{pmatrix}-f & +(1-f)\\ +f & -(1-f)\end{pmatrix}}_{\mathcal{L}_{pop}} \underbrace{\begin{pmatrix}\rho_{00}\\ \rho_{11}\end{pmatrix}}_{\vec{\rho}} \Rightarrow \vec{\rho}(t) = e^{\mathcal{L}_{pop} t}\vec{\rho}(0)$$

dot leer (ρ_{00}), besetzt (ρ_{11}), $f = f(\epsilon)$

BMS wird gut für schwache Kopplung $\Gamma(\epsilon) \to 0$

DCG wird gut für $t \to 0$, ist aber immer besser als BMS

1.4. Super-Operator Notation

BMS-MG:
$$\frac{d}{dt}\begin{pmatrix}\rho_{pop}\\ \rho_{coh}\end{pmatrix} = \underbrace{\begin{pmatrix}\mathcal{L}_{pop} & 0\\ 0 & \mathcal{L}_{coh}\end{pmatrix}}_{\mathcal{L}}\begin{pmatrix}\rho_{pop}\\ \rho_{coh}\end{pmatrix} \rightsquigarrow \rho(t) = e^{\mathcal{L}\cdot t}\rho(0)$$

Problem: Matrix von $\mathcal{L}$ per Hand zu konstruieren ist aufwändig

$\Rightarrow$ generelle Vektorisierung:

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

für eine bestimmte Ordnung der Basisvektoren kann das Tensorprodukt durch das Kronecker-Produkt dargestellt werden

$$A \otimes B = \begin{pmatrix} A_{11}B & \dots & A_{1N_A}\cdot B\\ \vdots & & \\ A_{N_A 1}B & \dots & A_{N_A N_A}\cdot B\end{pmatrix}$$

Zahlen, Matrix: $N_B \times N_B$

Vektoren: $N_A = 1$, $N_B = 1$

z.B.: $\rho = \begin{pmatrix}\rho_{00} & \rho_{01}\\ \rho_{10} & \rho_{11}\end{pmatrix} \Longleftrightarrow vec(\rho) = \begin{pmatrix}\rho_{00}\\ \rho_{01}\\ \rho_{10}\\ \rho_{11}\end{pmatrix}$

- $vec(A\rho) = \sum_{ijk}\underbrace{A_{ik}\cdot\rho_{kj}}_{(A\rho)_{ij}}\,|i\rangle \otimes |j\rangle$

$$\Rightarrow A\otimes \mathbb{1}\, vec(\rho) = \sum_{ij} \rho_{ij} \Big(\sum_{kl} A_{kl} |k\rangle \underbrace{\langle l|i\rangle}_{\delta_{il}}\Big) \otimes |j\rangle$$

$$= \sum_{ijk} \rho_{ij} A_{ki} |k\rangle \otimes |j\rangle \overset{k\leftrightarrow i}{=} \sum_{ijk} \rho_{kj} A_{ik} |i\rangle \otimes |j\rangle \quad \Big] =$$

- $$vec(\rho B) = \sum_{ijk} \rho_{ik} B_{kj} |i\rangle \otimes |j\rangle$$

$$\mathbb{1}\otimes B^T vec(\rho) = \sum_{ij} \rho_{ij} |i\rangle \otimes \Big(\sum_{kl} B_{lk} |k\rangle\langle l|j\rangle\Big) \quad \Big\} =$$

transponiert

$$\Rightarrow \boxed{vec(A\rho B) = A\otimes B^T \cdot vec(\rho)}$$

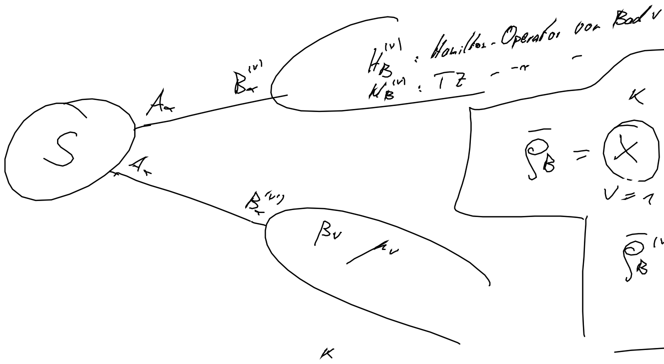
$$\dot{\rho} = -i[H_S,\rho] + \sum_\alpha \Big[L_\alpha \rho L_\alpha^\dagger - \frac{1}{2}\{L_\alpha^\dagger L_\alpha, \rho\}\Big] \Leftrightarrow \frac{d}{dt} vec(\rho) = \mathcal{L}\, vec(\rho)$$

$$\mathcal{L} = -i H\otimes \mathbb{1} + i\, \mathbb{1}\otimes H^T + \sum_\alpha \Big[L_\alpha \otimes (L_\alpha^\dagger)^T - \frac{1}{2} L_\alpha^\dagger L_\alpha \otimes \mathbb{1} - \frac{1}{2} \mathbb{1}\otimes (L_\alpha^\dagger L_\alpha)^T\Big]$$

- Spur $\hat{=}$ Summe der Diagonal-Elemente

$$Tr\{\rho\} = (vec(\mathbb{1}))^T \cdot vec(\rho) \quad \rightsquigarrow \text{Bsp: } (vec(\mathbb{1}))^T = (1,0,0,1)$$

2. Stationärer Quantentransport



$$\bar{\rho}_B = \bigotimes_{\nu=1}^{K} \bar{\rho}_B^{(\nu)}$$

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

$$H_I = \sum_\alpha A_\alpha \otimes B_\alpha = \sum_\alpha A_\alpha \otimes \underbrace{\sum_{\nu=1}^{K} B_\alpha^{(\nu)}}_{B_\alpha}$$

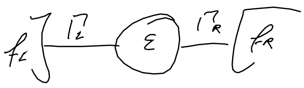
$$Tr\{\tilde{B}_\alpha^{(\nu)}(\tau) B_\beta^{(\mu)} \bar{\rho}_B\} = \begin{cases} Tr_\nu\{\tilde{B}_\alpha^{(\nu)}(\tau)\bar{\rho}_B^{(\nu)}\} \cdot Tr_\mu\{B_\beta^{(\mu)}\bar{\rho}_B^{(\mu)}\} = 0 & : \text{falls } \mu \neq \nu \\ Tr_\nu\{\tilde{B}_\alpha^{(\nu)}(\tau) B_\beta^{(\nu)} \bar{\rho}_B^{(\nu)}\} = C_{\alpha\beta}^{(\nu)}(\tau) & : \text{falls } \nu = \mu \end{cases}$$

⇝ keine Korrelationen zwischen verschiedenen Reservoiren (schwache Kopplung)

$$C_{\alpha\beta}(\tau) = \sum_{\nu=1}^{K} C^{(\nu)}_{\alpha\beta}(\tau)$$

$$\rightsquigarrow \boxed{\mathcal{L} = \mathcal{L}^{(0)} + \sum_\nu \mathcal{L}^{(\nu)} \qquad \mathcal{L}^{(0)}\rho \hat{=} -i\left[H_S, \rho\right]}$$

2.1. Bsp: SET



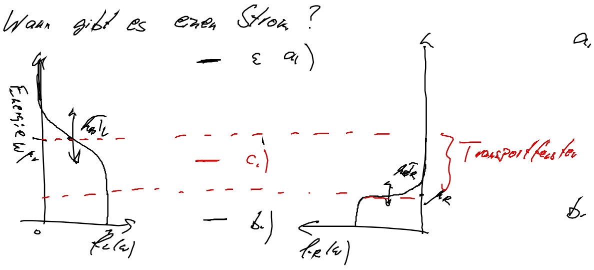
$$H = \varepsilon d^\dagger d + \sum_{\substack{k,\nu \\ \nu \in \{L,R\}}} \left(d^\dagger t_{k\nu} c_{k\nu} + h.c.\right) + \sum_{k\nu} \varepsilon_{k\nu} a_{k\nu}^\dagger a_{k\nu}$$

$$\mathcal{L}_{BGS} = \underbrace{\begin{pmatrix} -\Gamma_L \cdot f_L & +\Gamma_L(1-f_L) \\ +\Gamma_L \cdot f_L & -\Gamma_L(1-f_L) \end{pmatrix}}_{\mathcal{L}^{(L)}} + \underbrace{\begin{pmatrix} -\Gamma_R \cdot f_R & +\Gamma_R(1-f_R) \\ +\Gamma_R \cdot f_R & -\Gamma_R(1-f_R) \end{pmatrix}}_{\mathcal{L}^{(R)}}$$

$$\Gamma_\nu = \Gamma_\nu(\varepsilon) \qquad \Gamma_\nu(\omega) = 2\pi \sum_k |t_{k\nu}|^2 \delta(\omega - \varepsilon_{k\nu})$$

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

Wann gibt es einen Strom?



a.) $\varepsilon \gg \mu_L, \mu_R$ (tiefe T)

⇝ $f_L(\varepsilon) = f_R(\varepsilon) = 0$

⇝ dot entlädt ⇝ kein stat. Strom

b.) $\varepsilon \ll \mu_L, \mu_R$

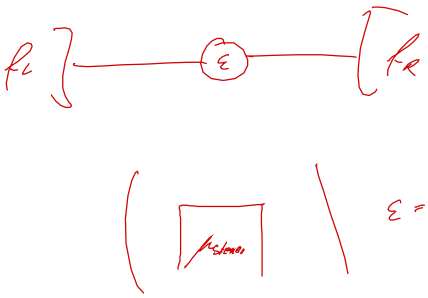
⇝ $f_\nu(\varepsilon) = 1$

⇝ dot ist beladen ⇝ kein stat. Strom

c.) $\mu_L > \varepsilon > \mu_R$

⇝ $f_L \to 1 \quad f_R \to 0$

⇝ dot wird von links geladen & entlädt nach rechts



$\varepsilon = \varepsilon(\mu_{Steuer})$

⇝ Transistor

⇝ stat. Lösung $\bar{\rho} = \begin{pmatrix} 1-\bar{f} \\ \bar{f} \end{pmatrix}$

$$\Gamma_\nu \geq 0 \qquad 0 \leq f_\nu \leq 1$$

$$\bar{f} = \frac{\Gamma_L \cdot f_L + \Gamma_R \cdot f_R}{\Gamma_L + \Gamma_R}$$

effektiver GG-Zustand
(weil das System so einfach ist)

therm. Parameter

geht immer falls

$$\mathcal{L}^{(\nu)} = \Gamma^{(\nu)} \left[\mathcal{L}_A + n^{(\nu)} \cdot \mathcal{L}_B \right] \quad \forall \nu$$

Kopplung

Superoperatoren $\rightsquigarrow \bar{\rho}^{(\nu)} = \bar{\rho}^{(\nu)}(\mathcal{L}_A, \mathcal{L}_B, n^{(\nu)})$

$$\mathcal{L}\bar{\rho} = 0 \iff 0 = \left[\sum_\nu \Gamma^{(\nu)}\right] \left[\mathcal{L}_A + \underbrace{\frac{\sum_\nu \Gamma^{(\nu)} \cdot n^{(\nu)}}{\sum_\nu \Gamma^{(\nu)}}}_{\bar{n}} \mathcal{L}_B \right] \bar{\rho} = 0$$

Spezialfall!

2.2. Phänomenologische Def. der Ströme

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

Energiebilanz

$$\frac{d}{dt} \langle E \rangle = \mathrm{Tr}\{ H_S \dot{\rho} \} = \mathrm{Tr}\{ H_S [-i H_S, \rho] \} + \sum_\nu \mathrm{Tr}\{ H_S (\mathcal{L}^{(\nu)} \rho) \}$$

$$= -i\, \mathrm{Tr}\{ H_S^2 \rho - \overbrace{H_S \rho H_S}^{\text{S}} \} + \sum_\nu I_E^{(\nu)}$$

$$\left(\sum_\nu \mathcal{L}^{(\nu)}\right)\bar{\rho} = 0$$

$$\rightsquigarrow \boxed{I_E^{(\nu)} = \mathrm{Tr}\{ H_S (\mathcal{L}^{(\nu)} \rho) \}} \xrightarrow{t\to\infty} \mathrm{Tr}\{ H_S (\mathcal{L}^{(\nu)} \bar{\rho}) \}$$

Energiestrom aus Reservoir ν

Teilchenbilanz: $[N_S, H_S] = 0$

$$\boxed{I_M^{(\nu)} = \mathrm{Tr}\{ N_S (\mathcal{L}^{(\nu)} \rho) \}}$$

Teilchenstrom aus Reservoir ν

im Langzeitlimes:

$$\bar{I}_{M/E}^{(L)} + \bar{I}_{M/E}^{(R)} = 0$$

Bsp: SET

$$I_E^{(L)}(t) = (1, 1) \begin{pmatrix} 0 & 0 \\ 0 & \varepsilon \end{pmatrix} \begin{pmatrix} -\Gamma_L \cdot f_L & +\Gamma_L (1-f_L) \\ +\Gamma_L \cdot f_L & -\Gamma_L (1-f_L) \end{pmatrix} \begin{pmatrix} \rho_{00}(t) \\ \rho_{11}(t) \end{pmatrix}$$

$\rightsquigarrow t\to\infty$: $\rho_{00} \to 1-\bar{f} \qquad \rho_{11} \to \bar{f}$

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

$\rightsquigarrow$ betrachte Ratengl.:

$$\dot{\rho}_{aa} = \sum_\nu \sum_b \gamma_{ab,ab}^{(\nu)} \rho_{bb} - \sum_\nu \sum_b \gamma_{ba,ba}^{(\nu)} \rho_{aa}$$

Rate von $b \to a$

$$\rho = \sum_a \rho_{aa} |a\rangle\langle a| + \sum_{ab:\, a\neq b} \rho_{ab} |a\rangle\langle b|$$

$$N_S = \sum_a N_a |a\rangle\langle a|$$
$$H_S = \sum_a E_a |a\rangle\langle a| \qquad \left([H_S, N_S] = 0 \right)$$

$$I_N^{(\nu)} = \sum_{a,b} \frac{(N_a - N_b)}{\Delta t} \underbrace{\Delta t \cdot \gamma^{(\nu)}_{ab,ab}\, \rho_{bb}}_{\text{WS für Sprung von } b \to a \text{ in } \Delta t} = \sum_{ab} (N_a - N_b)\, \gamma^{(\nu)}_{ab,ab}\, \rho_{bb}$$