

WdH

• Lösung der MG durch gekopp. Observablen

$$\text{Tr} \{ \dot{\hat{O}}; \hat{\rho} \} = -i \text{Tr} \{ \hat{O}; [H_S - \hat{H}] \} + \sum_j \text{Tr} \{ \hat{O}; [L_j \hat{\rho} L_j^\dagger - \frac{1}{2} L_j^\dagger L_j \hat{\rho} - \frac{1}{2} \hat{\rho} L_j^\dagger L_j] \}$$

$$\frac{d}{dt} \langle \hat{O}; \rangle = +i \langle [H, \hat{O}] \rangle + \sum_j \langle (L_j^\dagger \hat{O} L_j - \frac{1}{2} \{ \hat{O}, L_j^\dagger L_j \}) \rangle$$

$$\sum_j g_j \langle \hat{O}_j \rangle$$

"duale Mastergleichung" analog zum Kosselig-Bild
wirken auf \hat{O}

• partielle Spur

$$A = \sum_\alpha V_\alpha \otimes W_\alpha \quad \longrightarrow \quad \text{Tr}_V \{ A \} = \sum_\alpha V_\alpha \text{Tr} \{ W_\alpha \}$$

↙
wirkt nur auf V

$$\rho_{AB} \longrightarrow \begin{cases} \rho_A = \text{Tr}_B \{ \rho_{AB} \} \\ \rho_B = \text{Tr}_A \{ \rho_{AB} \} \end{cases}$$

falls $\rho_{AB} = \bar{\rho}_A \otimes \bar{\rho}_B$
 $\longrightarrow \text{Tr}_A \{ \rho_{AB} \} = \bar{\rho}_B$ & $\text{Tr}_B \{ \rho_{AB} \} = \bar{\rho}_A$

in Allgemeinen $\rho_{AB} \neq \rho_A \otimes \rho_B$ (Verschränkung)
 $\rho_A = \text{Tr}_B \{ \rho_{AB} \}$
 $\rho_B = \text{Tr}_A \{ \rho_{AB} \}$

Bsp.: $|\psi_{AB}\rangle = \frac{1}{\sqrt{2}} [|0\rangle_A \otimes |1\rangle_B + |1\rangle_A \otimes |0\rangle_B]$
 $\rho_{AB} = |\psi_{AB}\rangle \langle \psi_{AB}|$
 $\rho_A = \frac{1}{2} [|0\rangle\langle 0| + |1\rangle\langle 1|] \neq \rho_A^2$
 $\rho_A \otimes \rho_B \neq \rho_{AB}$

$A \hat{=}$ System $dn(A)$ klein
 $B \hat{=}$ Reservoir $dn(B) \rightarrow \infty$

• WW-Bild

$$\tilde{\rho}_{tot} = -i [\hat{H}_S + \hat{H}_B + \hat{H}_I, \rho_{tot}]$$

$$\tilde{\rho}_{tot} = -i [\tilde{H}_I(t), \tilde{\rho}_{tot}(t)]$$

$$\tilde{\rho} = e^{+i(\hat{H}_S + \hat{H}_B)t} \rho(t) e^{-i(\hat{H}_S + \hat{H}_B)t}$$

$$\tilde{H}_I(t) = e^{+i(\hat{H}_S + \hat{H}_B)t} \hat{H}_I e^{-i(\hat{H}_S + \hat{H}_B)t} \quad \left(\begin{array}{l} \text{o. B. d. d. } A_\alpha = A_\alpha^\dagger \\ \text{in } \hat{H}_I \text{ d. } B_\alpha = B_\alpha^\dagger \end{array} \right)$$

$$= \sum_\alpha e^{+i\epsilon_\alpha t} A_\alpha e^{-i\epsilon_\alpha t} \otimes e^{+i\epsilon_\alpha t} B_\alpha e^{-i\epsilon_\alpha t}$$

• formal integrieren $\int_0^t \dots dt'$

$$\tilde{\rho}_{tot}(t) = \rho_{tot}(0) - i \int_0^t [\tilde{H}_I(t'), \tilde{\rho}_{tot}(t')] dt'$$

wieder einsetzen

$$\tilde{\rho}_{tot} = -i [\tilde{H}_I(t), \rho_{tot}(0)] - \int_0^t dt' [\tilde{H}_I(t), [\tilde{H}_I(t'), \tilde{\rho}_{tot}(t')]] \quad \text{neu, noch ersetzt}$$

$$\tilde{\rho}_S = -i \text{Tr}_B \{ [\tilde{H}_I(t), \rho_{tot}(0)] \} - \int_0^t dt' \text{Tr}_B \{ [\tilde{H}_I(t), [\tilde{H}_I(t'), \tilde{\rho}_{tot}(t')] \} \}$$

① Born'sche Näherung $\tilde{\rho}_{tot}(t) = \rho_S(t) \otimes \bar{\rho}_B + \mathcal{O}(\lambda)$; $\tilde{H}_I = \mathcal{O}(\lambda)$
 $\rho_S^0 = \rho_S(0)$

$$\rho_S = -i \text{Tr}_B \{ [\tilde{H}_I(t), \rho_S^0 \otimes \bar{\rho}_B] \} - \int_0^t dt' \text{Tr}_B \{ [\tilde{H}_I(t), [\tilde{H}_I(t'), \rho_S(t') \otimes \bar{\rho}_B] \} \} + \mathcal{O}(\lambda^2)$$

$\mathcal{O}(\lambda)$ $\mathcal{O}(\lambda^2)$

↗ ↘
Nicht-Markov'sche Mastergleichung

kann zur Normalform gebracht werden

$$\begin{aligned} \text{Tr}_B \left\{ \sum_{\alpha} [\tilde{A}_{\alpha} \otimes \tilde{B}_{\alpha}, \rho_S^0 \otimes \rho_B^0] \right\} &= \sum_{\alpha} \left[\tilde{A}_{\alpha} \cdot \rho_S^0 \text{Tr}(\tilde{B}_{\alpha} \rho_B^0) - \rho_S^0 \tilde{A}_{\alpha} \text{Tr}(\rho_B^0 \tilde{B}_{\alpha}) \right] \\ &= \sum_{\alpha} [\tilde{A}_{\alpha}, \rho_S^0] \cdot \underbrace{\text{Tr}_B \left\{ e^{+i\lambda_{\alpha} t} \tilde{B}_{\alpha} e^{-i\lambda_{\alpha} t} \rho_B^0 \right\}}_{\text{falls } [\tilde{B}_{\alpha}, \rho_B^0] = 0} \quad \text{Res. ist 2. GG} \\ &= \text{Tr}_B \left\{ \tilde{B}_{\alpha} \rho_B^0 \right\} \end{aligned}$$

$$H_S \rightarrow H'_S = H_S + \sum_{\alpha} g_{\alpha} A_{\alpha} \quad g_{\alpha} \in \mathbb{R}$$

$$H_I \rightarrow H'_I = \sum_{\alpha} A_{\alpha} \otimes (\tilde{B}_{\alpha} - g_{\alpha} \mathbb{1}) \quad g_{\alpha} = \text{Tr}_B \left\{ \tilde{B}_{\alpha} \rho_B^0 \right\}$$

beschreiben

$$C_{\text{ops}}(t_1, t_2) = \text{Tr}_B \left\{ \tilde{B}_{\alpha}(t_1) \tilde{B}_{\beta}(t_2) \rho_B^0 \right\} = \text{Tr}_B \left\{ e^{-iH'_I(t_1-t_2)} \tilde{B}_{\alpha}(t_1) e^{+iH'_I(t_1-t_2)} \tilde{B}_{\beta}(t_2) \rho_B^0 \right\} = C_{\text{ops}}(t_1-t_2)$$

Zeit-korrelations-Funktion

$$\dot{\rho}_S = - \sum_{\alpha} \int_{\mathbb{R}} dt' \left\{ C_{\text{ops}}(t, t') [\tilde{A}_{\alpha}(t'), \tilde{A}_{\alpha}(t) \rho_S(t')] + C_{\text{ops}}(t', t) [\rho_S(t') \tilde{A}_{\alpha}(t'), \tilde{A}_{\alpha}(t)] \right\}$$

Nicht-Markovsche Mastergleichung

$$\dot{\rho}_S = \int_{\mathbb{R}} W(t, t') \rho_S(t') dt'$$

- geschlossene Integral-DGL
- nur für exakte $C_{\text{ops}}(t, t')$ lösbar
- erhält $\text{Tr}(\rho_S)$ & $\rho_S = \rho_S^\dagger$

② Markov Näherung (en)

$C_{\text{ops}}(t_1, t_2) = C_{\text{ops}}(t_1)$ fallen schnell ab

$$\dot{\rho}_S \approx \int_0^t W(t, t') dt' \rho_S(t') \approx \int_0^t W(t, t') dt' \rho_S(t)$$

1. Markov-Näherung
2. Markov-Näherung

BSP: $H_I = A \otimes \sum_{\alpha} (h_{\alpha} b_{\alpha} + h_{\alpha}^* b_{\alpha}^\dagger)$

Später \downarrow \uparrow Basis

$$C_{11}(t) = \text{Tr}_B \left\{ \underbrace{\sum_{\alpha} \left(h_{\alpha} b_{\alpha} e^{-i\lambda_{\alpha} t} + h_{\alpha}^* b_{\alpha}^\dagger e^{+i\lambda_{\alpha} t} \right)}_{\tilde{B}_1(t)} \left(\sum_{\beta} h_{\beta} b_{\beta} + h_{\beta}^* b_{\beta}^\dagger \right) \right\} \frac{e^{-\beta \sum_{\alpha} h_{\alpha} b_{\alpha}^\dagger h_{\alpha}}}{Z_B}$$

$$= \sum_k |k_n|^2 \left[\langle b_n b_n^\dagger \rangle e^{-i k_n \bar{v}} + \langle b_n^\dagger b_n \rangle e^{+i k_n \bar{v}} \right]$$

$$\frac{e^{-\beta \frac{\hbar^2 k_n^2}{2m}}}{Z_k} = \frac{1}{Z_k} e^{-\beta \hbar^2 k_n^2 / 2m}$$

$$\circ \text{Tr} \{ b_n e^{-\beta \hbar^2 k_n^2 / 2m} \} = \sum_{k=0}^{\infty} \langle k | b_n e^{-\beta \hbar^2 k_n^2 / 2m} | k \rangle = \sum_{k=0}^{\infty} \langle k | b_n | k \rangle e^{-\beta \hbar^2 k_n^2 / 2m} = 0$$

$$\circ \text{Tr} \{ b_n^2 e^{-\beta \hbar^2 k_n^2 / 2m} \} = 0$$

$$\circ \text{Tr} \left\{ b_n^\dagger b_n \frac{e^{-\beta \hbar^2 k_n^2 / 2m}}{Z_k} \right\} = \sum_{k=0}^{\infty} k \cdot \frac{e^{-\beta \hbar^2 k_n^2 / 2m}}{Z_k} = - \sum_{k=0}^{\infty} \frac{2}{\partial(\beta \hbar^2 k_n^2)} \ln \left(\sum_{k=0}^{\infty} e^{-\beta \hbar^2 k_n^2 / 2m} \right)$$

$$= \frac{2}{2(\beta \hbar^2)} \cdot \ln(1 - e^{-\beta \hbar^2})$$

$$\circ \text{Tr} \{ b_n b_n^\dagger \rho_B \} = \text{Tr} \left\{ \left(\frac{1}{2} + b_n^\dagger b_n \right) \rho_B \right\} = \frac{1}{1 - e^{-\beta \hbar^2}} = \frac{1}{e^{\beta \hbar^2} - 1} = h_B(\omega_k)$$

$$= 1 + h_B(\omega_k)$$

$$C_{11}(\bar{v}) = \sum_k |k_n|^2 \left[(1 + h_B(\omega_k)) e^{-i k_n \bar{v}} + h_B(\omega_k) e^{+i k_n \bar{v}} \right]$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \tilde{\gamma}(\omega) \left[(1 + h_B(\omega)) e^{-i \omega \bar{v}} + h_B(\omega) e^{+i \omega \bar{v}} \right] d\omega$$

spektrale (Kopplungs-) Dichte

$$\tilde{\gamma}(\omega) = \frac{1}{2\pi} \sum_k |k_n|^2 \delta(\omega - \omega_k) \geq 0$$

Freq. des h_B

Kopplungen ≥ 0

$$h_B(\omega) = - \ln(1 + h_B(\omega)) \quad \text{Prüfen}$$

analytisch fortsetzen

$$\tilde{\gamma}(-\omega) = - \tilde{\gamma}(\omega)$$

$$\int_{-\infty}^{+\infty} \tilde{\gamma}(\omega) [1 + h_B(\omega)] e^{-i \omega \bar{v}} d\omega$$

$$\gamma_{11}(\omega) = \int C(\bar{v}) e^{+i \omega \bar{v}} d\bar{v}$$

$$\gamma_{11}(\omega) = \tilde{\gamma}(\omega) [1 + h_B(\omega)] \geq 0$$

falls $\gamma_{11}(\omega)$ flach \Rightarrow Markov-Näherung ist gut

$$\dot{\hat{\rho}}_S = - \int_0^{\infty} \text{Tr}_B \left\{ [\hat{H}_I^\dagger(t), [\hat{H}_I(t-\bar{v}), \rho_S(t) \otimes \rho_B]] \right\} d\bar{v}$$

in Schröd-Bild

$$\dot{\hat{\rho}}_S = -i [\hat{H}_S, \hat{\rho}_S] - \left[\sum_{\alpha, \beta} \int_0^{\infty} C_{\alpha\beta}(\bar{v}) [\hat{A}_\alpha e^{-i \hat{H}_S \bar{v}} \hat{A}_\beta e^{+i \hat{H}_S \bar{v}} \hat{\rho}_S(t) + \text{h.c.}] \right] d\bar{v}$$

- zeit-lokal $\hat{\rho}_S = \sum \hat{\rho}_S$
- $\text{Tr} \{ \hat{\rho}_S \} = 1$ $\hat{\rho}_S = \hat{\rho}_S^\dagger$
- keiner i.A. keine Lindblad-Form

"Redfield-Gleichung" (off Markovsche Näherung!)

③ Säcular-Näherung notwendig um immer eine Lindblad-Form zu erhalten \rightarrow höchste Woche