WdH • TD der Mastergleichung

$$\bar\rho_B = \frac{e^{-\beta H_B}}{Z_B} \xrightarrow{\text{BMS}} \begin{array}{l} C_{\alpha\beta}(\tau) = C_{\beta\alpha}(-\tau - i\beta) \\ \gamma_{\alpha\beta}(-\omega) = \gamma_{\beta\alpha}(+\omega)\, e^{-\beta\omega} \end{array} \longrightarrow \bar\rho_S = \frac{e^{-\beta H_S}}{Z_S}$$

$$\mathcal{L}_{\text{BMS}}\, \bar\rho_S = 0$$

→ BMS ist eine Lindblad-Davies Abbildung

falls: $\bar\rho_B = \dfrac{e^{-\beta(H_B - \mu N_B)}}{Z_B} \xrightarrow[{[H_I, N_S + N_B] = 0}]{[H_S, N_S] = 0 \quad [H_B, N_B] = 0} \bar\rho_S = \dfrac{e^{-\beta(H_S - \mu N_S)}}{Z_S}$

- von-Neumann Entropie $\quad S(\rho) = -\mathrm{Tr}\{\rho \ln \rho\} = -\sum_n \rho_n \cdot \ln \rho_n$

  ρ_n: EW von ρ

  Bsp: $\rho = 1 \cdot |\psi_+\rangle\langle\psi_+| + 0\, |\psi_-\rangle\langle\psi_-|$

  $|\psi_+\rangle = \frac{1}{\sqrt2}\left[|0\rangle + |1\rangle\right] \qquad \rho = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

  $|\psi_-\rangle = \frac{1}{\sqrt2}\left[|0\rangle - |1\rangle\right]$

  $\rho_- = 0$

  $\rho_+ = 1 \qquad S(\rho) = 0$

- Spohn'sche Ungleichung $\quad \mathcal{L}\bar\rho = 0$

$$-\mathrm{Tr}\{(\mathcal{L}\rho)[\ln\rho - \ln\bar\rho]\} \geq 0$$

$$\frac{d}{dt} S(\rho) + \frac{d}{dt} S_{\text{res}} \geq 0 \qquad \text{2. HS}$$

- Coarse-graining

$$\tilde U = \mathbb{1} - i\int_0^t \tilde H_I(t')dt' - \underbrace{\int_0^t dt_1 \int_0^{t_1} dt_2\, \tilde H_I(t_1)\tilde H_I(t_2)}_{\int_0^t dt_1 \int_0^t dt_2\, \tilde H_I(t_1)\tilde H_I(t_2)\,\Theta(t_1 - t_2)} \pm \ldots$$

$$\mathrm{Tr}_B\{\tilde U(t)\, \rho_S^0 \otimes \bar\rho_B\, \tilde U^\dagger(t)\} \approx [\mathbb{1} + \mathcal{L}_t \cdot t + \ldots]\, \rho_S^0 \qquad \tau = t$$

$$\mathcal{L}_\tau \rho_S^0 = \frac{1}{\tau}\mathrm{Tr}_B\left\{\int_0^t H_I(t')dt'\, \rho_S^0 \int_0^t H_I(t')dt' - \int_0^t dt_1 \int_0^{t_1} dt_2\, H_I(t_1) H_I(t_2)\, \rho_S^0 - \int_0^t dt_1 \int_0^{t_1} dt_2\, \rho_S^0\, H_I(t_2) H_I(t_1)\right\}$$

$$\Theta(t_1 - t_2) = \frac{1}{2}(1 + \mathrm{sgn}(t_1 - t_2))$$

=> $\mathcal{L}_\tau$ ist eine Lindblad Form

$\mathcal{L}_\tau$ ist auch gut für kurze Zeiten

$$\rho_S(t) = e^{\mathcal{L}_t \cdot t} \rho_S^0$$

$e^{\mathcal{L}_\tau \cdot t} \rho_S^0$ ist immer eine valide DM

"dynamisches coarse-graining"

BMS: 3 Näherungen: + schw. Kopplung, schnell abf. Korrel.-Funktionen
+ lange Zeiten

DCG: - schwache $(t \cdot H_I)$. abfallende Korrelationsfunktionen

$$\frac{d}{dt}\rho_S(t) = \underbrace{\left[\left(\frac{d}{dt} e^{\mathcal{L}_t \cdot t}\right) e^{-\mathcal{L}_t\cdot t}\right]}_{\mathcal{L}^{DGB}(t)} \underbrace{e^{+\mathcal{L}_t\cdot t}\rho_S^0}_{\rho_S(t)}$$

i. A. keine Lindblad Form

$$\sum_{ab} |a\rangle\langle a| e^{+iH_S t} A_\alpha e^{-iH_S t}|b\rangle\langle b|$$

$[H_B, \rho_B] = 0$

$$\rightsquigarrow C_{\alpha\beta}(t_1-t_2) = \frac{1}{2\pi}\int d\omega\, \gamma_{\alpha\beta}(\omega)\, e^{-i\omega(t_1-t_2)}$$

$$C_{\alpha\beta}(t_1-t_2)\,\mathrm{sgn}(t_1-t_2) = \frac{1}{2\pi}\int \sigma_{\alpha\beta}(\omega)\, e^{-i\omega(t_1-t_2)}\, d\omega$$

$$A_\alpha^{\omega,\tau} = \int_0^\tau dt\, \tilde A_\alpha(t)\, e^{-i\omega t}$$

CG-Mastergleichung (τ fixiert)

$$\dot{\tilde\rho}_S = -i\left[\frac{1}{2i\tau}\frac{1}{2\pi}\sum_{\alpha\beta}\int d\omega\, \sigma_{\alpha\beta}(\omega)\, A_\alpha^{\omega,\tau} A_\beta^{-\omega,\tau}, \tilde\rho_S\right]$$

$$+\frac{1}{\tau}\sum_{\alpha\beta}\frac{1}{2\pi}\int d\omega\, \gamma_{\alpha\beta}(\omega)\left[A_\beta^{-\omega,\tau}\tilde\rho_S A_\alpha^{+\omega,\tau} - \frac{1}{2}\left\{A_\alpha^{+\omega,\tau}A_\beta^{-\omega,\tau},\tilde\rho_S\right\}\right]$$

nutze $\int_0^\tau e^{-i\alpha_x \cdot t}\, dt = \tau\cdot e^{-i\alpha_x \tau/2}\cdot \mathrm{sinc}\left(\frac{\alpha_x\tau}{2}\right)$ $\qquad \mathrm{sinc}(x) = \frac{\sin(x)}{x}$

$$\lim_{\tau\to\infty} \tau\cdot\mathrm{sinc}\left[\frac{\tau}{2}(\Omega_a-\omega)\right]\mathrm{sinc}\left[\frac{\tau}{2}(\Omega_b-\omega)\right] = 2\pi\cdot\delta_{\Omega_a,\Omega_b}\cdot\delta(\Omega_a-\omega)$$

$$\boxed{\lim_{\tau\to\infty}\mathcal{L}_\tau^{CG} = \mathcal{L}_{BMS}}$$

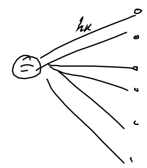
1.3.6. Beispiel: Spin-Boson-Modell

Verteilung der Kopplungsstärke $\quad$ Verteilung der Bad-Energien

$$\Gamma(\omega) = 2\pi\sum_k |h_k|^2\,\delta(\omega-\omega_k) \quad \text{spektrale Dichte}$$

$H_S = \Omega\cdot\sigma^z + T\sigma^x \qquad H_B = \sum_k \omega_k b_k^\dagger b_k$

$$H_I = \underbrace{\sigma^z}_{A_1}\otimes\underbrace{\sum_k\left(h_k b_k + h_k^* b_k^\dagger\right)}_{B_1}$$



- exakt lösbar für $T=0$: $[H_S,H_I]=0$ "pure dephasing"
- $\mathrm{Tr}\{\tilde B_1(\tau)\cdot B_1\, \bar\rho_B\} = \sum_k |h_k|^2\left[[1+n_B(\omega_k)]\cdot e^{-i\omega_k\tau} + n_B(\omega_k)\cdot e^{+i\omega_k\tau}\right]$

$= C(\tau)$

$$= \frac{1}{2\pi}\int_0^\infty \left[\Gamma(\omega)\,[1+n_B(\omega)]\,e^{-i\omega\tau} + n_B(\omega)\, e^{+i\omega\tau}\,\Gamma(\omega)\right]d\omega = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\underbrace{\tilde\Gamma(\omega)\,[1+n_B(\omega)]}_{\gamma(\omega)}\, e^{-i\omega\tau}\, d\omega$$

$$\tilde\Gamma(-|\omega|) = -\Gamma(+|\omega|)$$

häufige Annahme: $\tilde\Gamma(\omega) = \Gamma_0\cdot\omega\, e^{-|\omega|/\omega_c}$

ohmsche SD $\qquad$ cutoff

• exakte Lösung $T=0$

$$\tilde{A}_1(t) = e^{+iH_S t}\sigma_z e^{-iH_S t} = \sigma_z \qquad \tilde{B}_1(t) = \sum_k \left(h_k b_k e^{-i\omega_k t} + h_k^* b_k^\dagger e^{+i\omega_k t}\right)$$

harte Polaron-Trafo

$$U_P = \exp\Big\{-\sigma^z \underbrace{\sum_k\left(\frac{h_k}{\omega_k}b_k - \frac{h_k^*}{\omega_k}b_k^\dagger\right)}_{B}\Big\} \qquad U = \cosh(B) - \sinh(B)\cdot\sigma^z \rightsquigarrow U_P^{-1} = U_P^\dagger$$

$$\boxed{\begin{aligned}&\bullet\ U_P \sigma^z U_P^\dagger = \sigma^z\\ &\bullet\ U_P b_k U_P^\dagger = b_k + \left[+\sigma^z \frac{h_k^*}{\omega_k} b_k^\dagger, b_k\right] = b_k - \frac{h_k^*}{\omega_k}\cdot\sigma^z\end{aligned}}$$

$$e^A B e^{-A} = \sum_{n=0}^\infty \frac{1}{n!}[A,B]_n \qquad [A,B]_0 = B, \quad [A,B]_n = [A,[A,B]_{n-1}]$$

$$\bullet\ U_P \sigma^\pm U_P^\dagger = e^{\pm 2\sum_k\left(\frac{h_k^*}{\omega_k}b_k^\dagger - \frac{h_k}{\omega_k}b_k\right)}\sigma^\pm$$

$$U_P H U_P^\dagger = \Omega\cdot\sigma^z + \sigma^z \sum_k\left(h_k b_k + h_k^* b_k^\dagger - \frac{|h_k|^2}{\omega_k}\cdot\sigma^z\cdot 2\right) + \sum_k \omega_k\left(b_k^\dagger - \frac{h_k}{\omega_k}\sigma^z\right)\left(b_k - \frac{h_k^*}{\omega_k}\sigma^z\right)$$

$$= \Omega\sigma^z - \sum_k \frac{|h_k|^2}{\omega_k} + \sum_k \omega_k b_k^\dagger b_k$$

Spin-Boson-Entkopplung $\overset{?}{\circ}$

$$\langle\sigma^\alpha\rangle = \mathrm{Tr}\{e^{+iHt}\sigma^\alpha e^{-iHt}\rho_0\} = \dots$$

$$\vdots$$

$$\boxed{\tilde{\rho}_{01}(t) = \exp\Big\{-\frac{4}{\pi}\int_0^\infty \Gamma(\omega)\frac{\sin^2(\omega t/2)}{\omega^2}\cdot\coth\left(\frac{\beta\omega}{2}\right)d\omega\Big\}\rho_{01}(0)}$$

"Dekohärenz"

$$\tilde{\rho}_{00}(t) = \rho_{00}(0) \qquad \tilde{\rho}_{11}(t) = \rho_{11}(0)$$

• jetzt: BMS Mastergleichung ($T\neq 0$)

$$\gamma(\omega) = \Gamma(\omega)[1+n_B(\omega)] \longrightarrow \sigma(\omega)$$

$$H_S|\pm\rangle = E_\pm|\pm\rangle \qquad E_\pm = \pm\sqrt{\Omega^2+T^2}$$

$$\gamma_{-+,-+} = \Gamma\left(+2\sqrt{\Omega^2+T^2}\right)\left[1+n_B\left(+2\sqrt{\Omega^2+T^2}\right)\right]|\langle-|\sigma^z|+\rangle|^2 \xrightarrow{T\to 0} 0$$

$$\gamma_{+-,+-} = \Gamma(\quad''\quad)\, n_B\left(+2\sqrt{\Omega^2+T^2}\right)|\langle-|\sigma^z|+\rangle|^2 \xrightarrow{T\to 0} 0$$

$$\gamma_{--,++} = \gamma(0)\langle-|\sigma^z|-\rangle\langle+|\sigma^z|+\rangle = \gamma_{++,--}$$

↳ in BMS

$$\frac{d}{dt}\rho_{--} = +\gamma_{-+,-+}\rho_{++} - \gamma_{+-,+-}\rho_{--}$$

$$\frac{d}{dt}\rho_{++} = +\gamma_{+-,+-}\rho_{--} - \gamma_{-+,-+}\rho_{++}$$

$$\frac{d}{dt}\rho_{-+} = -i(E_- - E_+ + \sigma_{--} - \sigma_{++})\rho_{-+} + \underbrace{\left(\gamma_{--,++} - \frac{\gamma_{-+,-+}+\gamma_{+-,+-}}{2}\right)}_{\leq 0}\rho_{-+}$$

$$= \eta\cdot\rho_{-+}$$

$$\frac{d}{dt}\begin{pmatrix}\rho_{--}\\ \rho_{++}\\ \rho_{-+}\\ \rho_{+-}\end{pmatrix} = \underbrace{\begin{pmatrix}-\gamma_{+-,+-} & +\gamma_{-+,-+} & 0 & 0\\ +\gamma_{+-,+-} & -\gamma_{-+,-+} & 0 & 0\\ 0 & 0 & \eta & 0\\ 0 & 0 & 0 & \eta^*\end{pmatrix}}\begin{pmatrix}\rho_{--}\\ \rho_{++}\\ \rho_{-+}\\ \rho_{+-}\end{pmatrix}$$

$$= \begin{pmatrix}\mathcal{L}_{pop} & 0\\ 0 & \mathcal{L}_{coh}\end{pmatrix}$$

$\Rightarrow$ $\bar{\rho}_S$ stimmt mit exakter Lösung überein für $T = 0$

$\Rightarrow$ zeitliche Dynamik stimmt nicht ganz

<u>Ausblick</u> $\bar{\rho}_S = \mathrm{Tr}_B \left\{ \frac{e^{-\beta H_{tot}}}{Z_{tot}} \right\}$