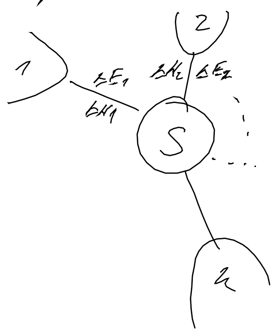
Wdh. • Symmetrien in der KGF $\Leftrightarrow$ Fluktuationstheoreme : stochastische Formulierung des 2. HS

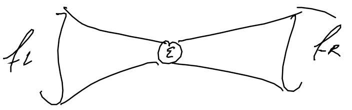


$$\lim_{t\to\infty} \frac{\overbrace{P_{+\Delta N,+\Delta E}(t)}^{P_{+\Delta_i S}}}{\underbrace{P_{-\Delta N,-\Delta E}(t)}_{P_{-\Delta_i S}}} = e^{-\sum_{\nu=1}^{N}\beta_\nu(\Delta E_\nu - \mu_\nu \Delta N_\nu)} = e^{\Delta_i S}$$

Trajektorien mit $\Delta_i S > 0$ sind viel wahrscheinlicher als $\Delta_i S < 0$

vorher: $\dot{S}_i = \frac{d}{dt} S[\rho_S] - \sum_\nu \beta_\nu \left[\bar{I}_E^{(\nu)} - \mu_\nu \bar{I}_M^{(\nu)}\right] \xrightarrow{t\to\infty} -\sum_\nu \beta_\nu \left[\bar{I}_E^{(\nu)} - \mu_\nu \bar{I}_M^{(\nu)}\right]$

• starke Kopplung $\to$ nicht-gilt mehr
+ nichtwechselwirkende Modelle sind für Elektronen exakt lösbar



Transmission $0 \le T(\omega) \le 1$

Ströme $I_M = \frac{1}{2\pi}\int T(\omega)\,[f_L(\omega) - f_R(\omega)]\,d\omega$

$I_E = \frac{1}{2\pi}\int T(\omega)\cdot\omega\,[f_L(\omega) - f_R(\omega)]\,d\omega$

$\dot{S}_i \to (\beta_R - \beta_L)\cdot I_E + (\beta_L\mu_L - \beta_R\mu_R) I_M \ge 0$ (schwache Kopplung)

$\to \frac{1}{2\pi}\int T(\omega)\, \underbrace{[(\beta_R-\beta_L)\omega + (\beta_L\mu_L - \beta_R\mu_R)]\,[f_L(\omega) - f_R(\omega)]}_{\ge 0}\, d\omega \underset{\substack{\uparrow \\ \text{starke Kopplung}}}{\ge} 0$

4.12. Polaron Mastergleichungen

4.12.1. Ein bosonisches Reservoir

$$H = H_S + \sum_k \omega_k \Big[b_k^\dagger + \frac{h_k}{\omega_k}\cdot \underset{\substack{\downarrow\\ \text{System-Operator}}}{S}\Big]\Big[b_k + \frac{h_k^*}{\omega_k} S\Big]$$
$$= H_S' + \sum_k \omega_k b_k^\dagger b_k + S\sum_k (h_k b_k + h_k^* b_k^\dagger)$$

$B^\dagger B$ ist immer positiv

$\langle\psi|B^\dagger B|\psi\rangle = \sum_n \langle\psi|B^\dagger|n\rangle\langle n|B|\psi\rangle$
$= \sum_n |\langle n|B|\psi\rangle|^2 \ge 0$

$H_S' = H_S + \sum_k \frac{|h_k|^2}{\omega_k} S^2$
$= H_S + \frac{1}{2\pi}\int \frac{\Gamma(\omega)}{\omega}\,d\omega\cdot S^2$

$$\boxed{U_P = \exp\Big[S\sum_k\Big(\frac{h_k^*}{\omega_k} b_k^\dagger - \frac{h_k}{\omega_k} b_k\Big)\Big]}$$
Polaron-Trafo (Lang-Firsov-Trafo) unitär

$S = S^\dagger$

• $U_P S U_P^\dagger = S$

• $U_P b_k U_P^\dagger = b_k - \frac{h_k^*}{\omega_k}\cdot S$ • $U_P b_k^\dagger U_P^\dagger = b_k^\dagger - \frac{h_k}{\omega_k}\cdot S$

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

$= B + [A,B] + \dots$

$$H' = U_P H U_P^\dagger = U_P H_S U_P^\dagger + \sum_k \omega_k b_k^\dagger b_k$$

Kopplung steckt hier drin

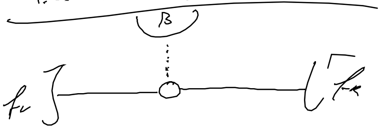
$$= \underbrace{\mathrm{Tr}_B\left\{U_P H_S U_P^\dagger \frac{e^{-\beta \sum_k \omega_k b_k^\dagger b_k}}{Z}\right\}}_{H_S'} + \underbrace{\left[U_P H_S U_P^\dagger - \mathrm{Tr}_B\left\{U_P H_S U_P^\dagger \frac{e^{-\beta\sum_k \omega_k b_k^\dagger b_k}}{Z}\right\}\right]}_{H_I'} + \underbrace{\sum_k \omega_k b_k^\dagger b_k}_{H_B'}$$

→ Ableitung Standard Mastergleichung im Polaronbild

+ Polaron-Trafo nimmt nicht alle Terme der Störungstheorie mit, aber beinhaltet alle Ordnungen

\- technisch schwierig

4.2.2. Phononen-gekoppelter SET



$$H = \underbrace{\varepsilon d^\dagger d + \sum_k \sum_\nu \varepsilon_{k\nu} c_{k\nu}^\dagger c_{k\nu} + \sum_k \sum_\nu \left(t_{k\nu} c_{k\nu} d^\dagger + h.c.\right)}_{SET} + \underbrace{d^\dagger d \sum_{q=1}^{Q} \left(h_q a_q + h_q^* a_q^\dagger\right)}_{H_{SET,ph}} + \underbrace{\sum_q \omega_q a_q^\dagger a_q}_{H_B^{ph}}$$

$$U_P = \exp\Big\{\underbrace{d^\dagger d}_{S} \underbrace{\sum_q \left(\frac{h_q^*}{\omega_q} a_q^\dagger - \frac{h_q}{\omega_q} a_q\right)}_{A}\Big\} = e^{d^\dagger d \hat{A}} = \mathbb{1} + d^\dagger d \left(e^{\hat{A}} - \mathbb{1}\right) \rightarrow U_P d U_P^\dagger = d \cdot e^{-\hat{A}}$$

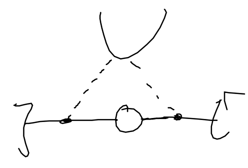
$$U_P d^\dagger U_P^\dagger = d^\dagger e^{+\hat{A}}$$

$$U_P H U_P^\dagger = H' = \left(\varepsilon - \sum_q \frac{|h_q|^2}{\omega_q}\right) d^\dagger d + \sum_{k\nu} \varepsilon_{k\nu} c_{k\nu}^\dagger c_{k\nu} + \sum_q \omega_q a_q^\dagger a_q$$

$$+ \underbrace{\sum_{k\nu} \left(t_{k\nu} d\, c_{k\nu}^\dagger e^{-\hat{A}} + t_{k\nu}^* c_{k\nu} d^\dagger e^{+\hat{A}}\right)}_{H_I}$$

vorher

=>



jeder elektronische Sprung kann Phononen anregen oder vernichten

- $t_{k\nu}$ perturbativ h_q nicht perturbativ

$$\rho_B' = \bar{\rho}_B^L \, \bar{\rho}_B^R \, \bar{\rho}_B^{ph}$$

$$B_{1\nu} = \sum_k t_{k\nu} c_{k\nu}^\dagger e^{-A} \qquad B_{2\nu} = \sum_k t_{k\nu}^* c_{k\nu} e^{+A}$$

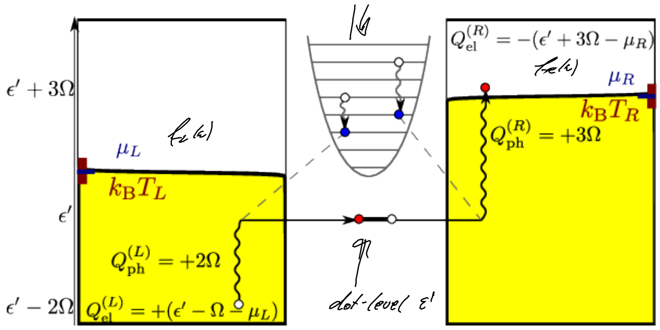
$$\frac{1}{2\pi} \int \Gamma_\nu(\omega) f_\nu(-\omega) \cdot e^{-i\omega\tau} d\omega$$

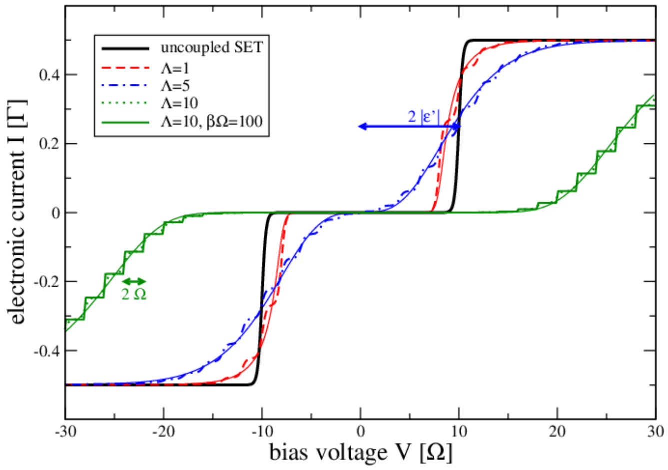
$$C_{12}^\nu(\tau) = \langle B_{1\nu}(\tau) B_{2\nu} \rangle_{\rho_B'} = C_{12,el}^\nu(\tau) C_{12,ph}(\tau)$$

$$C_{21}^\nu(\tau) = \dots = C_{21,el}^\nu(\tau) C_{21,ph}(\tau)$$

$$\frac{1}{2\pi} \int \Gamma_\nu(\omega) [1 - f_\nu(\omega)] e^{-i\omega\tau} d\omega$$

$$C_{12,ph}(\tau) = \exp\left\{\sum_q \frac{|h_q|^2}{\omega_q^2} \left[e^{-i\omega_q \tau}\left(1 + n_B(\omega_q)\right) + e^{+i\omega_q\tau} \cdot n_B(\omega_q) - \left(1 + 2 n_B(\omega_q)\right)\right]\right\} = C_{21,ph}(\tau)$$





4.3. Bosonische Reaktionskoordinaten - Abbildungen

4.3.1. Bosonische Bog.-Trafo

lineare Trafo, welche die Kommutator-Relationen respektiert

$$a_k = \sum_q u_{kq} b_q + v_{kq} b_q^\dagger$$

Bosonen; $u_{kq}, v_{kq} \in \mathbb{C}$

$$[a_k, a_{k'}^\dagger] = \delta_{kk'} \quad [a_k, a_{k'}] = 0 \iff [b_q, b_{q'}^\dagger] = \delta_{qq'} \quad [b_q, b_{q'}] = 0$$

$$u_{kq} = (U)_{kq} \qquad v_{kq} = (V)_{kq}$$

(symplektische Trafo:

$$U U^\dagger - V V^\dagger = \mathbb{1} \qquad U V^T - V U^T = 0$$

)

Spezialfall: • $v_{kq} = 0 \rightsquigarrow U U^\dagger = \mathbb{1} \to U$ ist unitär

• $u_{kq} = \frac{1}{2}\left(\frac{\alpha_k}{\beta_q} + \frac{\beta_q}{\alpha_k}\right)\Lambda_{kq} \qquad v_{kq} = \frac{1}{2}\left(\frac{\alpha_k}{\beta_q} - \frac{\beta_q}{\alpha_k}\right)\Lambda_{kq}$

$$\sum_q \Lambda_{kq} \Lambda_{k'q} = \delta_{kk'}$$