Real-Time RG: Nonequilibrium properties of open quantum systems

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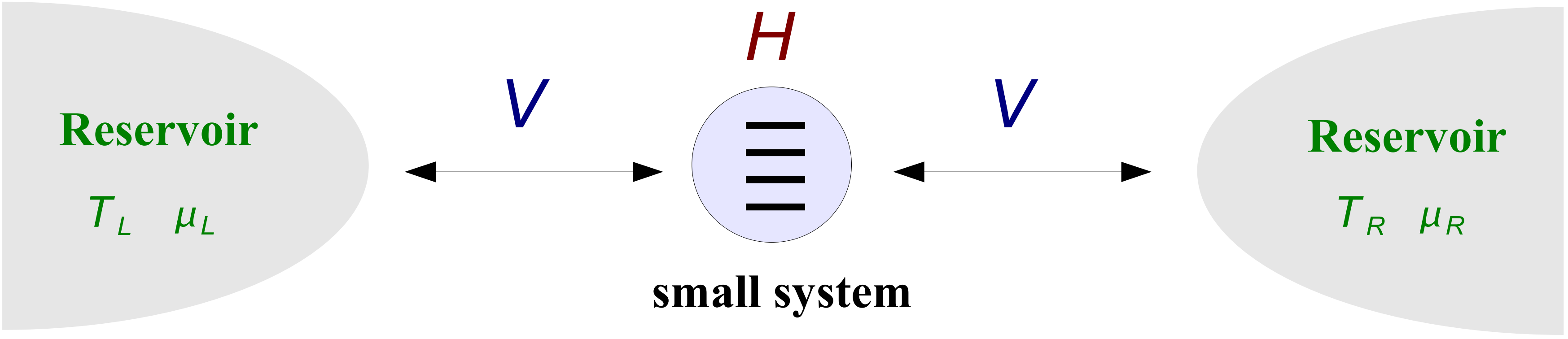
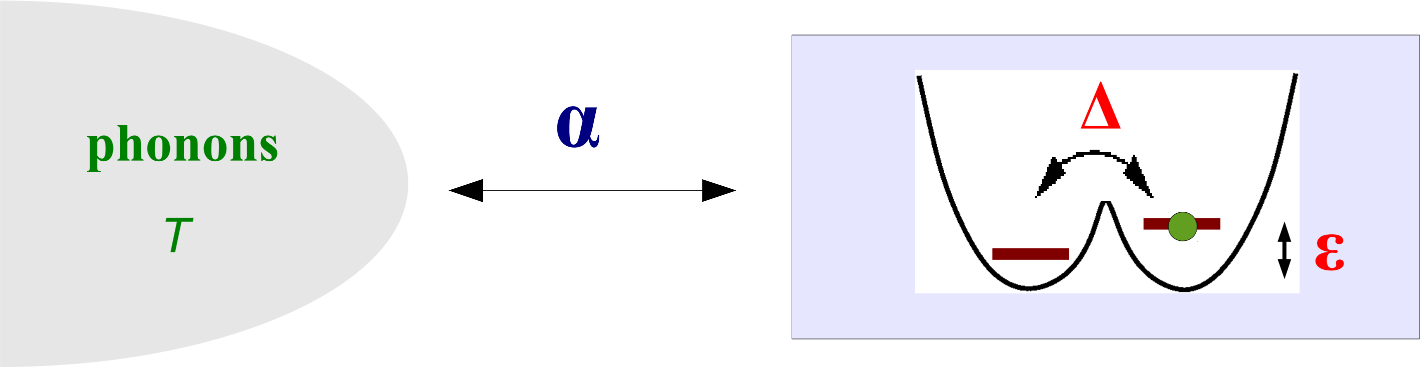


- $H_{tot} = H + H_{res} + V$
- expand in system-bath interaction V
- calculate reduced density matrix of the system $\rho(t) = Tr_{res} \; \rho_{tot}(t)$
- calculate observables (e.g. current) $\langle I_\alpha \rangle (t) = Tr_{tot} \; I_\alpha \; \rho_{tot}(t)$

Ohmic spin boson model: Energy fluctuations



$$H_{res} = \sum_k \omega_k a_k^\dagger a_k$$

$$H = \epsilon/2 \ \sigma_z - \Delta/2 \ \sigma_x$$

$$V = \frac{1}{2} \sigma_z \sum_k \alpha_k (a_k + a_k^\dagger)$$

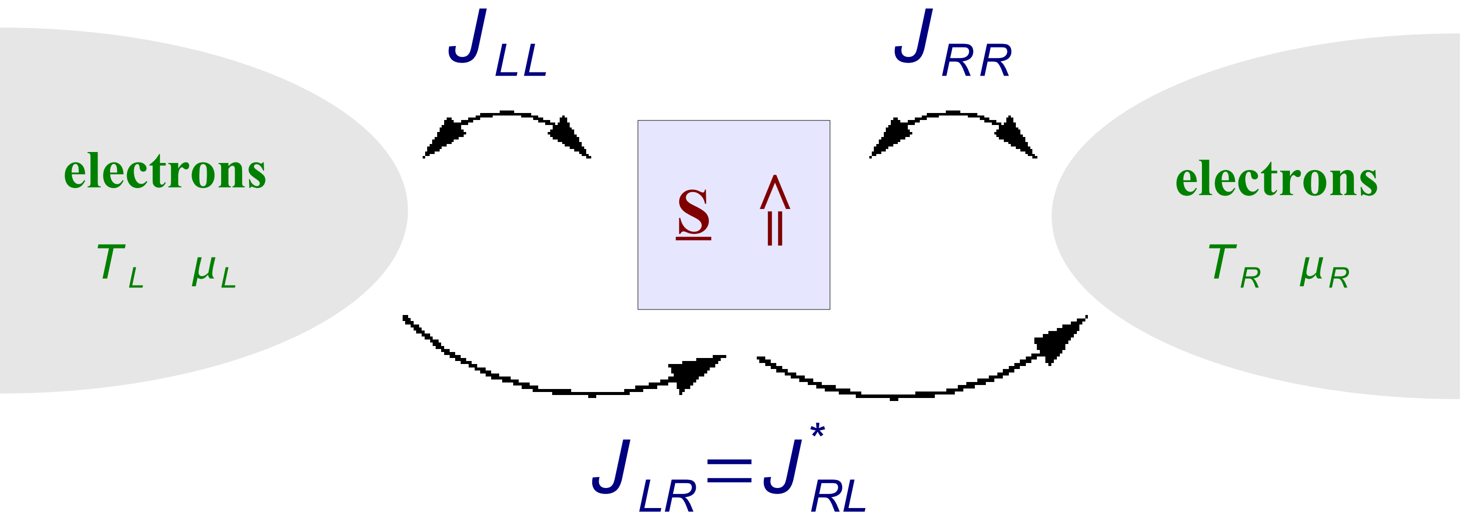
$$\rho(\omega) = \sum_k \alpha_k^2 \delta(\omega - \omega_k) = 2\alpha\omega\theta(\omega)$$

ohmic case

expand in

$$\boxed{\alpha \ll 1}$$

Nonequilibrium Kondo model: Spin fluctuations



J_{LL}

J_{RR}

electrons

$T_L \quad \mu_L$

$\underline{S} \quad \Uparrow$

electrons

$T_R \quad \mu_R$

$J_{LR} = J^*_{RL}$

$$H^L_{res} = \sum_k \epsilon_{L\sigma k} a^\dagger_{L\sigma k} a_{L\sigma k} \qquad H = h \; S_z \qquad H^R_{res} = \sum_k \epsilon_{R\sigma k} a^\dagger_{R\sigma k} a_{R\sigma k}$$

$$V = \sum_{\alpha\alpha'} \frac{J_{\alpha\alpha'}}{\rho_0} \underline{S} \sum_{kk'} \sum_{\sigma\sigma'} \frac{1}{2} a^\dagger_{\alpha\sigma k} \underline{\sigma}_{\sigma\sigma'} a_{\alpha'\sigma' k'} = \sum_{\alpha\alpha'} \frac{J_{\alpha\alpha'}}{\rho_0} \underline{S} \; \underline{s}^{\alpha\alpha'}_{res}$$

expand in $\boxed{|J_{\alpha\alpha'}| \ll 1}$

Formalism: Basic ideas

von Neumann equation: $i\frac{d}{dt}\rho_{tot}(t) = [H_{tot}, \rho_{tot}(t)] = L_{tot}\rho_{tot}(t)$

$L_{tot} = [H_{tot}, \cdot]$ → Liouville superoperator, acts in Liouville space = space of all operators

➡ $\rho_{tot}(t) = e^{-iL_{tot}t}\rho_{tot}(0)$

Initial condition: $\rho_{tot}(t=0) = \rho_{t=0}\prod_\alpha \rho_\alpha^{(eq)}$ $\qquad \rho_\alpha^{(eq)} = e^{-\beta_\alpha(H^\alpha_{res}-\mu_\alpha N^\alpha_{res})}/Z_\alpha$

effective von Neumann equation: $\rho(t) = Tr_{res}\ \rho_{tot}(t)$ integrate out reservoirs

$L_{tot} = L^{(0)} + L_{res} + L_V$ $\qquad L_{res}=[H_{res},\cdot]$

↓ ↓

$$i\frac{d}{dt}\rho(t) = Tr_{res}L_{tot}\rho_{tot}(t) = Tr_{res}(L^{(0)}+L_{res}+L_V)\rho_{tot}(t)$$

$$= L^{(0)}\rho(t) + Tr_{res}L_V e^{-i(L^{(0)}+L_{res}+L_V)t}\rho_{t=0}\prod_\alpha \rho_\alpha^{(eq)}$$

↙

expand + Wick theorem + resummation

Kinetic equation ; Quantum Boltzmann equation:

$$i\frac{d}{dt}\rho(t) = \underbrace{L^{(0)}\rho(t)}_{\text{coherence}} + \int_0^t dt' \underbrace{\Sigma(t-t')}_{\text{dissipation , memory term}} \rho(t')$$

Effective Liouvillian:

$$L(t-t') = L^{(0)}\delta(t-t'-0^{+}) + \Sigma(t-t')$$

$$i\frac{d}{dt}\rho(t) = \int_0^t dt' \; L(t-t') \; \rho(t')$$

$L(t-t')$ → response function

→ defined for t > t'

Formal solution in Fourier space:

exponentially
decaying for Im E > 0

$$\rho(E) = \int_0^\infty dt \;\; e^{iEt} \;\; \rho(t) \qquad\qquad L(E) = \int_0^\infty dt \;\; e^{iEt} \;\; L(t)$$

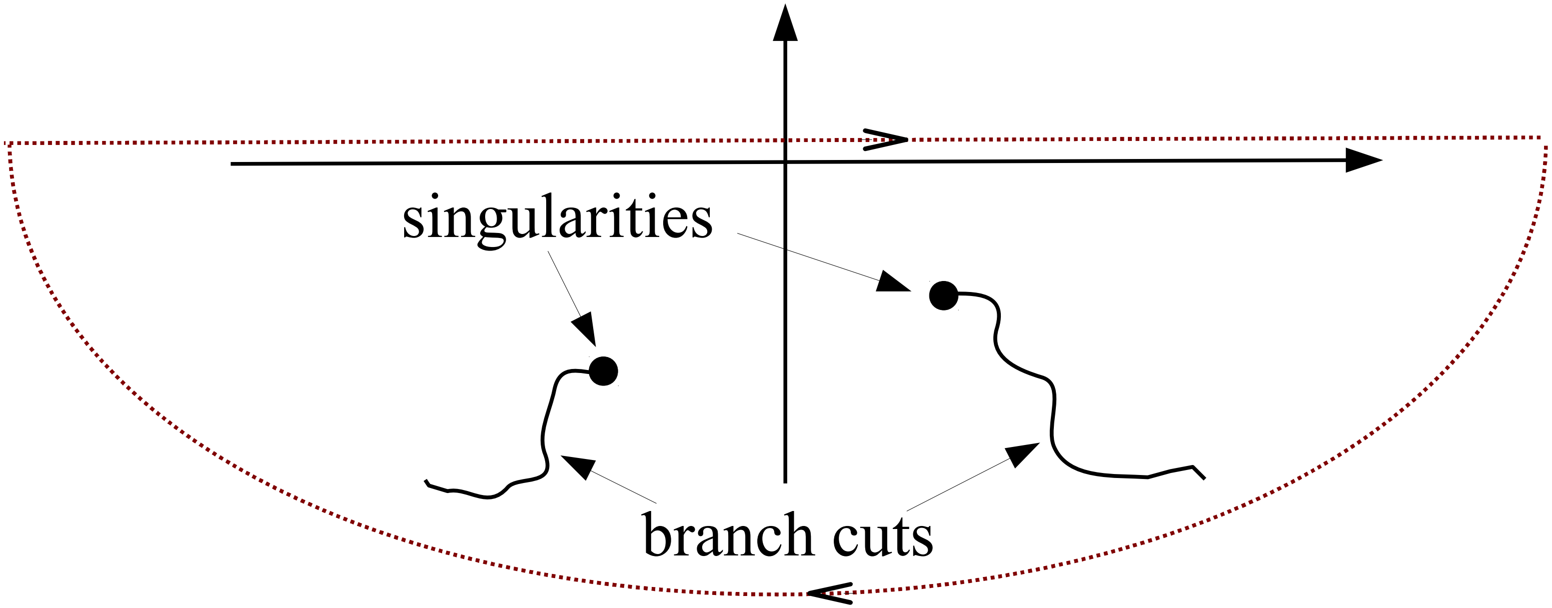
analytic functions in the
upper half of the complex plane

$$i\frac{d}{dt}\rho(t) = \int_0^t dt' \;\; L(t-t') \;\; \rho(t') \qquad => \qquad E\rho(E) - i\rho_{t=0} = L(E)\rho(E)$$

$$=> \qquad \boxed{\rho(E) = \frac{i}{E-L(E)} \;\; \rho_{t=0}} \qquad \boxed{\rho(t) = \frac{i}{2\pi}\int_{-\infty+i0^+}^{\infty+i0^+} dE \;\; \frac{e^{-iEt}}{E-L(E)} \;\; \rho_{t=0}}$$

close in lower half: t > 0

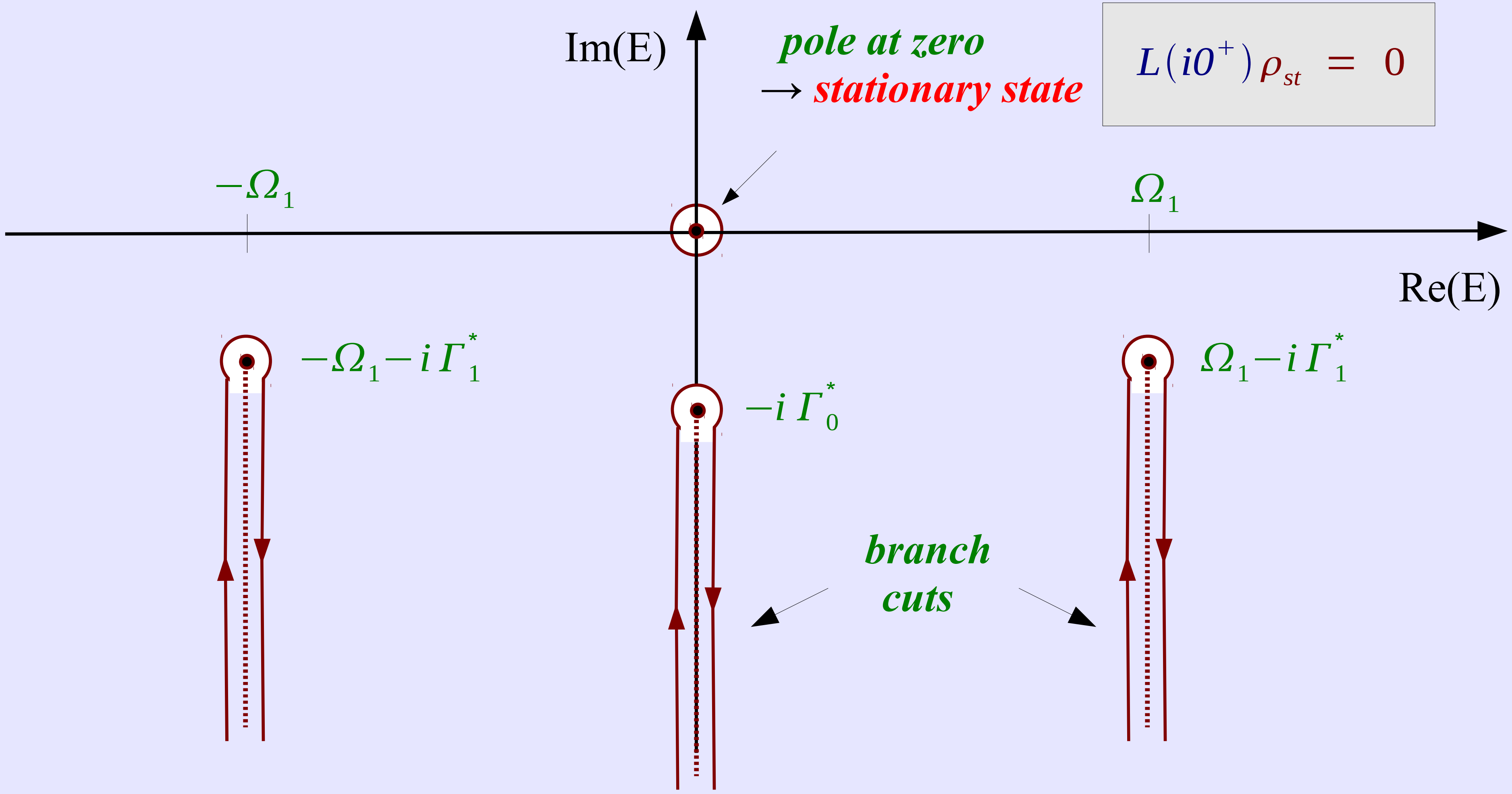
Close integration contour in lower half:



Analytic continuation:

(D → ∞ , T=0)

$$\rho(t) = \frac{i}{2\pi}\int_{-\infty+i0^+}^{\infty+i0^+} dE\, \frac{e^{-iEt}}{E-L(E)}\, \rho_{t=0}$$



pole at zero
→ *stationary state*

$$L(i0^+)\,\rho_{st} = 0$$

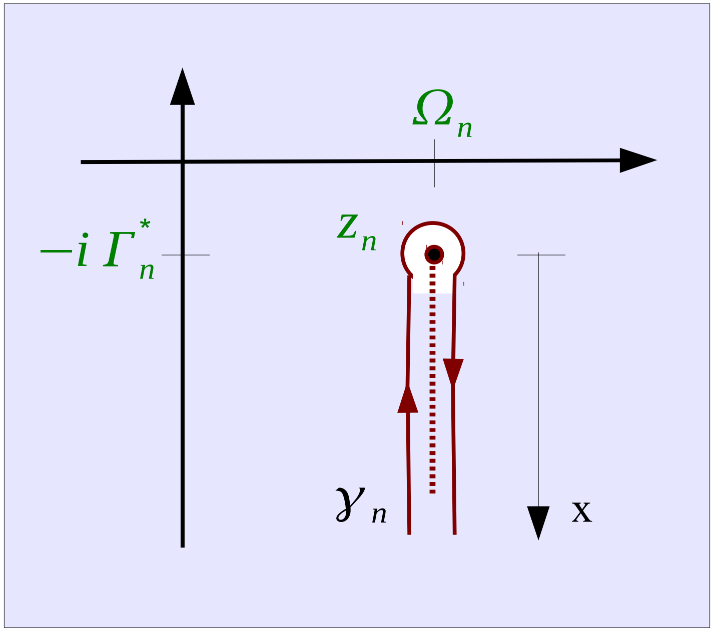
branch cuts

$$F_1(t)^\dagger e^{i\Omega_1 t} e^{-\Gamma_1^* t}$$

$$F_0(t) e^{-\Gamma_0^* t}$$

$$F_1(t) e^{-i\Omega_1 t} e^{-\Gamma_1^* t}$$

Single contribution:



$$z_n = \Omega_n - i\,\Gamma^*_n$$

$$E = z_n - i\,x \pm 0^+$$

$$0 < x < \infty$$

$$dE = -i\,dx$$

$$\frac{i}{2\pi}\int_{\gamma_n} dE \quad \frac{e^{-iEt}}{E-L(E)} \quad \rho_{t=0} \quad =$$

$$= e^{-i\Omega_n t} e^{-\Gamma^*_n t} \quad \underbrace{\frac{1}{2\pi}\int_0^\infty dx \quad e^{-xt}\left\{\frac{1}{z_n - i\,x - L(z_n - i\,x + 0^+)} - \frac{1}{z_n - i\,x - L(z_n - i\,x - 0^+)}\right\}}_{F_n(t)} \quad \rho_{t=0}$$

exponentially decaying => analytical progress possible in the long-time limit

$$\boxed{\rho(t) = \rho_{st} + \sum_n F_n(t) \; e^{-i\Omega_n t} \; e^{-\Gamma^*_n t} \; \rho_{t=0}}$$

General consideration about the E-dependence of ρ(E) and L(E)

ρ(E) vs. L(E): $\rho(E) = \frac{i}{E-L(E)}\,\rho_{t=0}$

→ perturbative expansion of L(E) avoids secular terms $\sim \left(\frac{1}{E-L^{(0)}}\right)^k \sim t^k$

Secular terms in L(E): L(E) itself contains terms $\sim\left(\frac{1}{E-z_n}\right)^k$

→ can be avoided by self-consistent perturbation theory for L(E)

→ all singularities of ρ(E) lie in lower half of complex plane

Logarithmic terms in L(E):

$$\boxed{L(E) = L_\Delta(E) + E\,L'(E)}$$

$\sim \Delta \neq E$ physical scale

dimensionless

$L_\Delta(E), L'(E)$ → slowly varying logarithmic functions

→ high energies: $\left(\alpha \ln\frac{D}{E-z_n}\right)^k$ low energies: $\left(\alpha \ln\frac{E-z_n}{E-z_m}\right)^k$

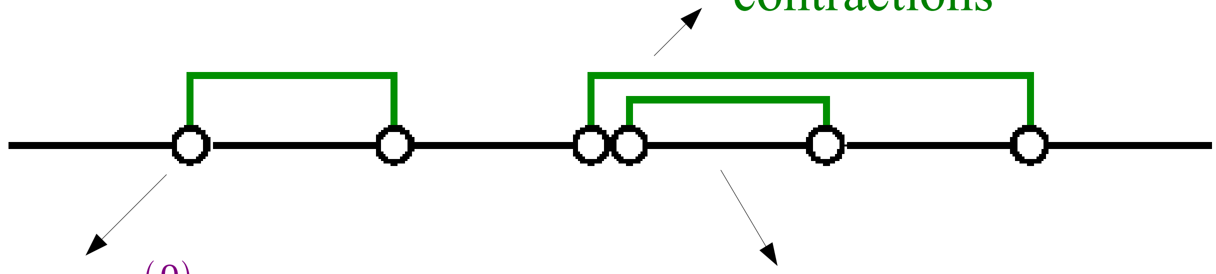
→ treat by renormalization group (RG)

Quantum field theory in Liouville space

expand in L_V + Wick theorem =>

reservoir contractions → contain $f_\alpha(\omega)$ $\rho_{\alpha\sigma}(\omega)$

$\rho(E)$ →



vertices $G^{(0)}$

→ superoperators

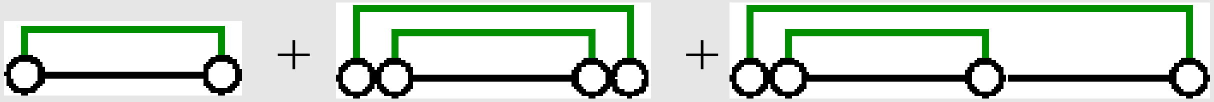
→ contain interaction V

local propagation $\dfrac{1}{E+\bar{\mu}_{1\ldots n}+\bar{\omega}_{1\ldots n}-L^{(0)}}$

→ superoperators

→ contain E , μ_α , $L^{(0)}=[H,\cdot]$

$\Sigma(E)$ =



+ ...

= sum over connected diagrams ≡ “self-energy”

$$L(E) = L^{(0)} + \Sigma(E)$$

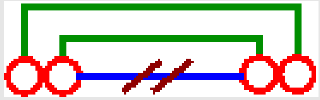
use perturbative expansion for L(E) and not for

$$\rho(E) = \frac{i}{E-L(E)}\rho_{t=0}$$

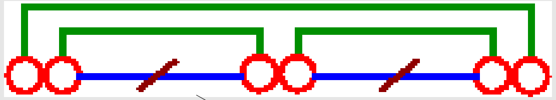
E-flow scheme of real-time renormalization group (E-RTRG)

$L(E)$ → contains divergencies $\left(\frac{1}{E-z_n}\right)^k$, $\left(\ln\frac{D}{E-z_n}\right)^k$, $\left(\ln\frac{E-z_n}{E-z_m}\right)^k$

$\frac{\partial^2}{\partial E^2}L(E) =$



$+$

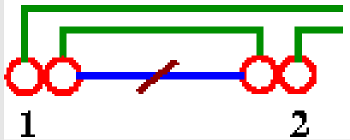


$+ \; .....$

full propagators

effective vertices

$\frac{\partial}{\partial E}G_{12}(E) =$



$+ \; .....$

(1) full propagators → resum self-energy insertions

(2) consider derivatives → renormalization group (RG)

(3) effective vertices → resum vertex corrections

(1) + (2) + (3) => well-defined power series in $G_{12}(E)$ for all energies:

$$\frac{1}{E-z_n}\cdot\left(c_1 G^2 + c_2 G^3 + c_3 G^4 + \ldots\right)$$

→ controlled truncation possible if $G(E) << 1$

RG equations : $L(E) = L_\Delta(E) + E L'(E)$

$$\frac{\partial L_\Delta(E)}{\partial E} = \sum_n \frac{1}{E-z_n} \Psi^n_{L_\Delta}\{L_\Delta, L', G\}$$

$$\frac{\partial L'(E)}{\partial E} = \sum_n \frac{1}{E-z_n} \Psi^n_{L'}\{L_\Delta, L', G\}$$

$$\frac{\partial G(E)}{\partial E} = \sum_n \frac{1}{E-z_n} \Psi^n_{G}\{L_\Delta, L', G\}$$

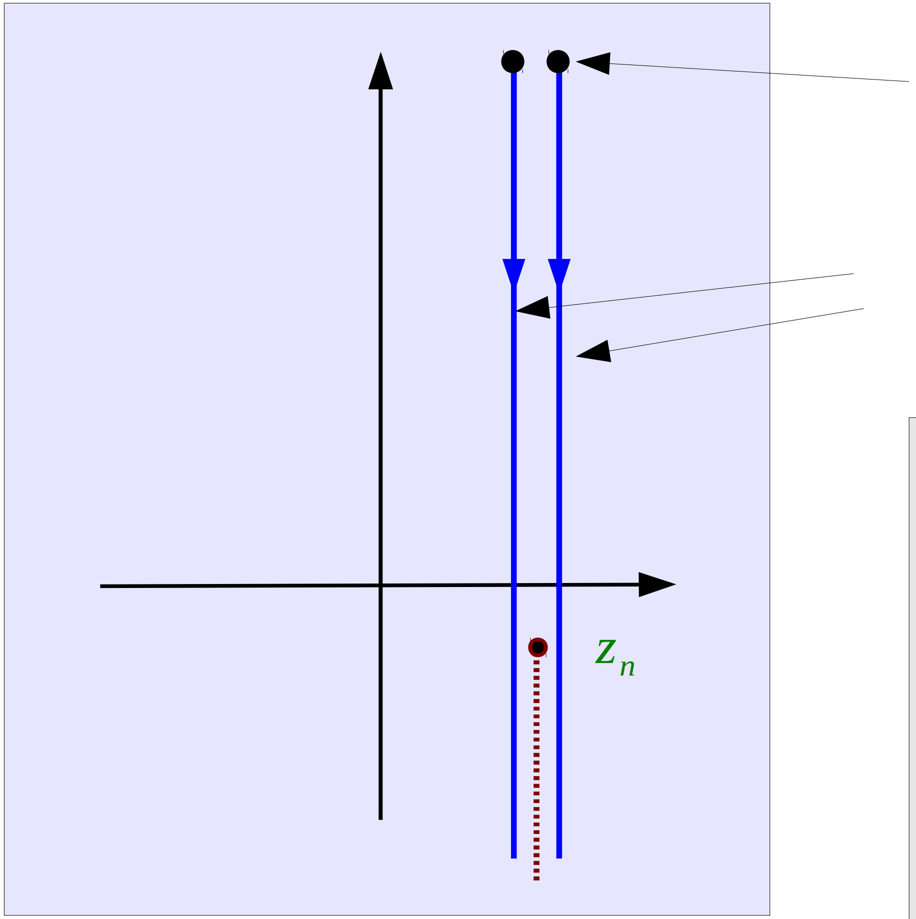
$\Psi^n_{L_\Delta}$, $\Psi^n_{L'}$, Ψ^n_G → functionals which do not contain any logarithmic divergencies at **low and high** energies

→ expand in $G(E) \ll 1$ (**weak coupling**) and truncate at certain order

→ all logarithmic powers are resummed up to a certain order :

$\alpha^k \ln^k$ → leading order (1-loop)
$\alpha^k \ln^{k-1}$ → sub-leading order (2-loop)
$\alpha^k \ln^{k-2}$ → sub-sub-leading order (3-loop)   etc.

Solve RG equations along certain path in complex plane :



start at high energies
(perturbative initial condition)

solve RG equation along these paths

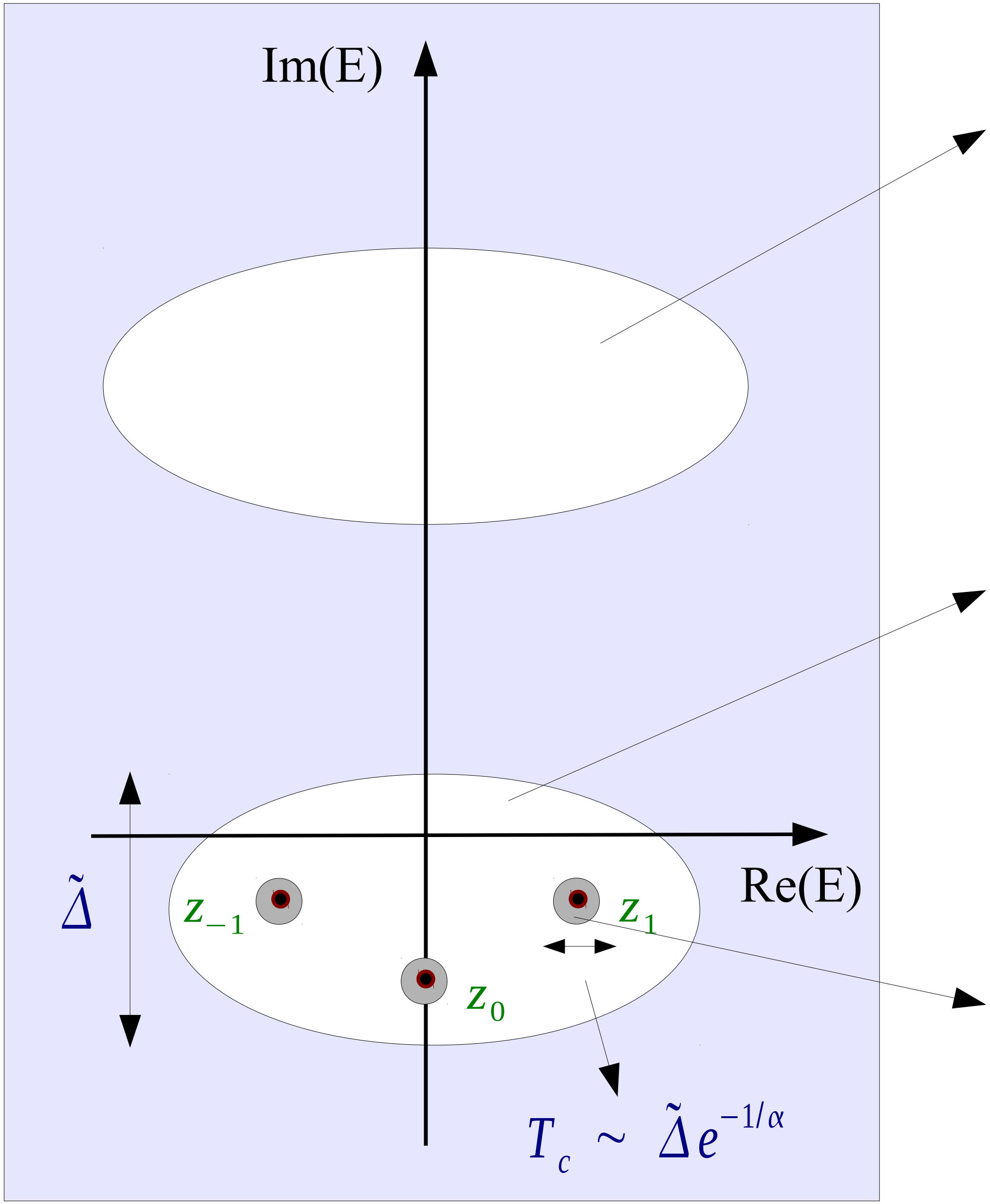
→ allows for an analytic continuation into the lower half of the complex plane

→ allows for the determination of the position of the branching points / poles

→ allows for a convenient choice of the shape of the branch cuts

→ allows for analytical solutions in weak coupling $G \ll 1$

Analytical solution in different energy regimes



High energies :

$|E| \sim 1/t \gg |z_n|$ neglect all z_n

$$L_\Delta(E), L'(E) \approx L_\Delta(\frac{1}{t}), L'(\frac{1}{t})$$

Small/intermediate energies :

$$\tilde{\Delta} \sim |z_n| \geq |E| \sim 1/t \gg T_c$$

expand in $\alpha \ln \frac{\tilde{\Delta}}{E-z_n} \ll 1$

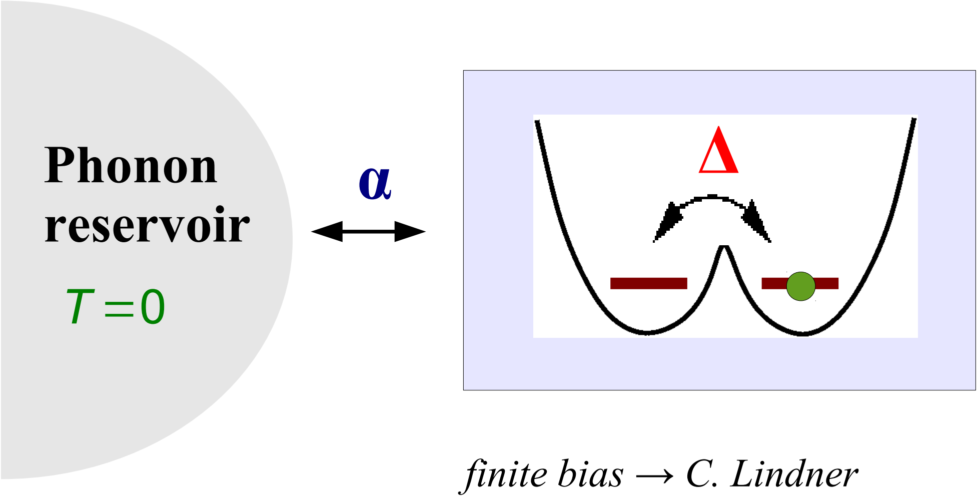
Exponentially small energies :

$|E| \sim 1/t \leq T_c$ $\quad \alpha \ln \frac{\tilde{\Delta}}{E-z_n} \sim 1$

neglect all other branching points

Ohmic spin boson model: weak damping

Kashuba & Schoeller,
PRB 87, 201402(R) (2013)



$$H_{tot} = \sum_k \omega_k a_k^\dagger a_k - \frac{1}{2}\Delta\,\sigma_x + V$$

$$V = \frac{1}{2}\sigma_z \sum_k \alpha_k (a_k + a_k^\dagger)$$

$$\rho(\omega) = \sum_k \alpha_k^2 \delta(\omega - \omega_k) = 2\alpha\omega\theta(\omega) \quad \text{ohmic}$$

finite bias → C. Lindner
Tu 15:45, TT45.8

$\rightarrow$ $\boxed{\varepsilon = T = 0 \qquad \alpha \ll 1}$

Energy scales :

$$D \gg \tilde{\Delta} = \Omega \gg \Gamma^* \gg T_c$$

reservoir
band width

renormalized tunneling
= oscillation frequency

$$\tilde{\Delta} = \Delta\left(\frac{\Delta}{D}\right)^{\frac{\alpha}{1-\alpha}}$$

relaxation rate

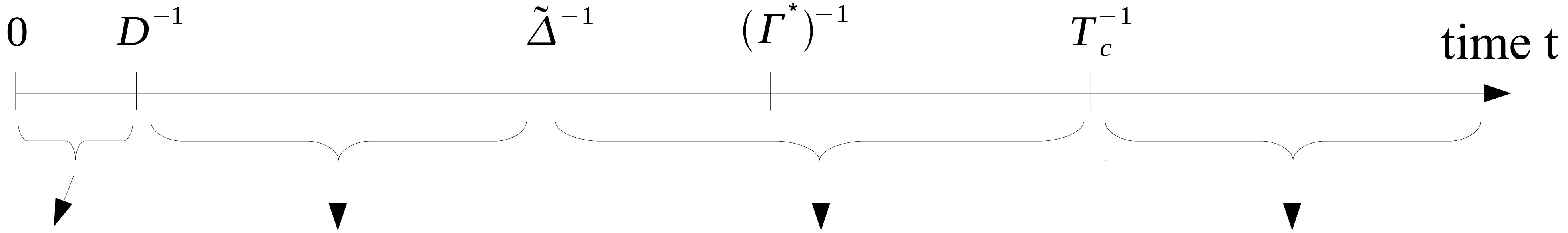
$$\Gamma^* = \pi\alpha\tilde{\Delta}$$

exponentially small
energy scale

$$T_c \sim \tilde{\Delta}\, e^{-\frac{1}{\alpha}}$$

Effective spin dynamics : $\langle\sigma_{x,z}\rangle(t) = ?$ $\langle\sigma_y\rangle(0) = 0$

$$D \gg \tilde{\Delta} = \Delta\left(\frac{\Delta}{D}\right)^{\frac{\alpha}{1-\alpha}} = \Omega \gg \Gamma^* = \pi\alpha\tilde{\Delta} \gg T_c \sim \tilde{\Delta} e^{-\frac{1}{\alpha}}$$



non-universal
perturbative
in α

short times

sum up $(\alpha\ln(Dt))^k$

$$\langle\sigma_z\rangle(t) = \langle\sigma_z\rangle(0)$$
$$\langle\sigma_x\rangle(t) = \left(\frac{1}{Dt}\right)^{2\alpha}\langle\sigma_x\rangle(0)$$

long times

sum up $(\alpha\ln(D/\Delta))^k$

$\rightarrow$ $\tilde{\Delta} = \Delta\left(\frac{\Delta}{D}\right)^{\frac{\alpha}{1-\alpha}}$

expand in $\alpha\ln(\tilde{\Delta}t) \ll 1$

exponentially large times

$\alpha\ln(\tilde{\Delta}t) \sim O(1)$

sum up $(\alpha\ln(\tilde{\Delta}t))^k$

$$s(t) = (1+\alpha\ln(\tilde{\Delta}t))^{-2}\cdot$$
$$\cdot(1-\ln(1+\alpha\ln(\tilde{\Delta}t)))^{-2}$$

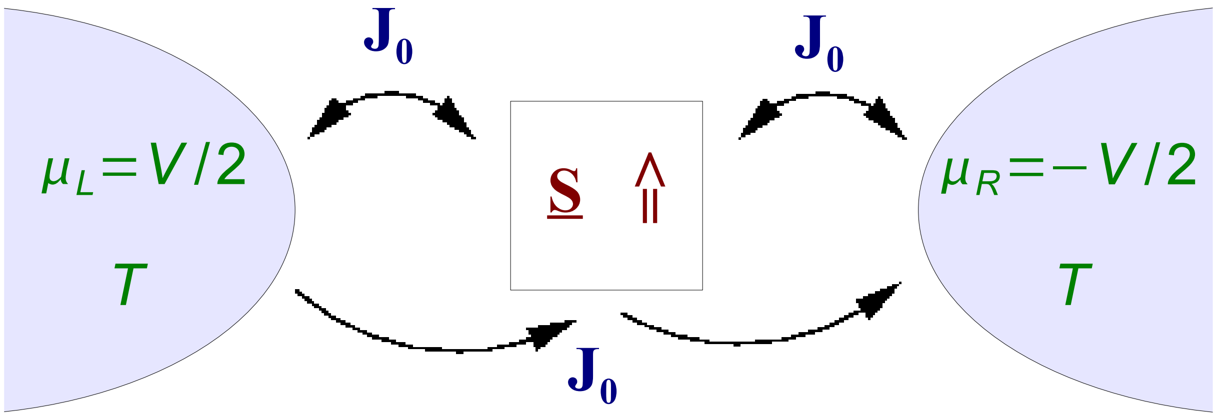
$$\langle\sigma_z\rangle(t) = \cos(\tilde{\Delta}t)e^{-\frac{\Gamma^*}{2}t}\langle\sigma_z\rangle(0) - \frac{2\alpha}{(\tilde{\Delta}t)^2}e^{-\Gamma^* t}\langle\sigma_z\rangle(0)$$

$$\langle\sigma_x\rangle(t) = \frac{\tilde{\Delta}}{\Delta} - \frac{\tilde{\Delta}}{\Delta}e^{-\Gamma^* t} + \left(\frac{\tilde{\Delta}}{\Delta}\right)^2 e^{-\Gamma^* t}\langle\sigma_x\rangle(0) - 2\alpha\frac{s(t)}{(\Delta t)^2}\cos(\tilde{\Delta}t)e^{-\frac{\Gamma^*}{2}t}\langle\sigma_x\rangle(0)$$

stationary state

Nonequilibrium Kondo model

Schoeller & Reininghaus, PRB 80, 045117 (2009)
Pletyukhov, Schuricht & Schoeller, PRL 104, 106801 (2010)
Pletyukhov & Schoeller, PRL 108, 260601 (2012)
Reininghaus, Pletyukhov & Schoeller, PRB 90, 085121 (2014)



$$H_{tot} = H_{res} + V$$

$$H_{res} = \sum_{\alpha=L,R} \sum_{\sigma=\uparrow,\downarrow} \sum_k \epsilon_{\alpha\sigma k} a^\dagger_{\alpha\sigma k} a_{\alpha\sigma k}$$

$$V = \frac{J_0}{\rho_0} \underline{S} \cdot \underline{s}_{res} \qquad J_0 \ll 1$$

spin 1/2, 1 channel, h=0

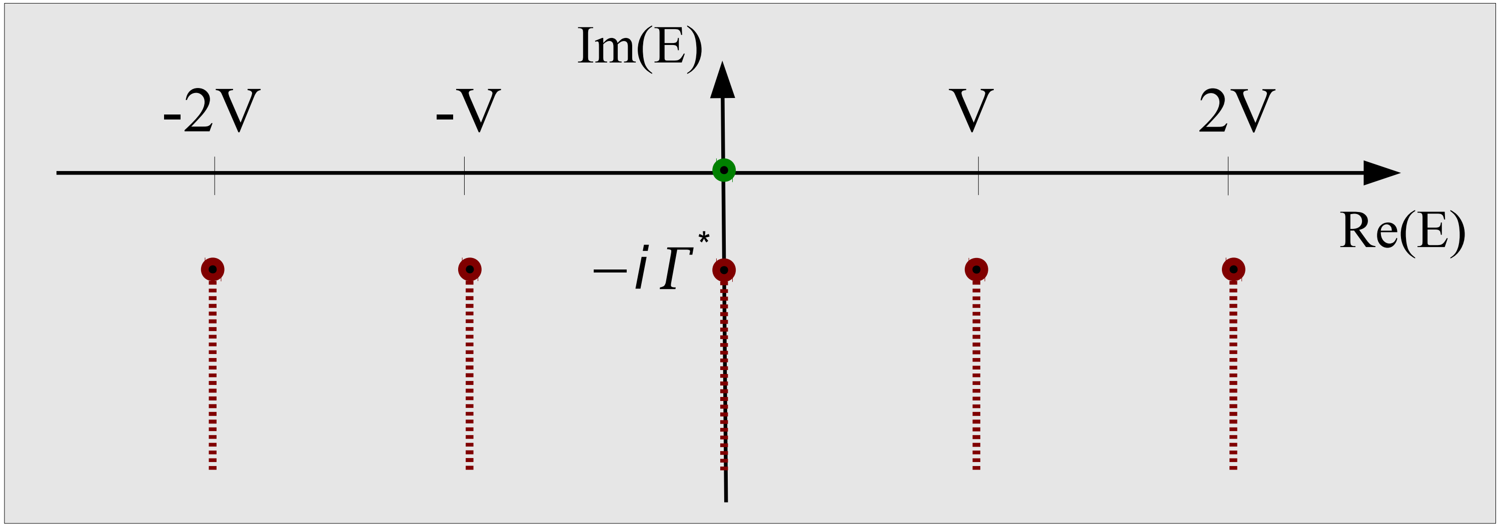
Strong coupling :

$$T, V \leq T_K = D e^{-1/(2J_0)}$$

stationary quantities

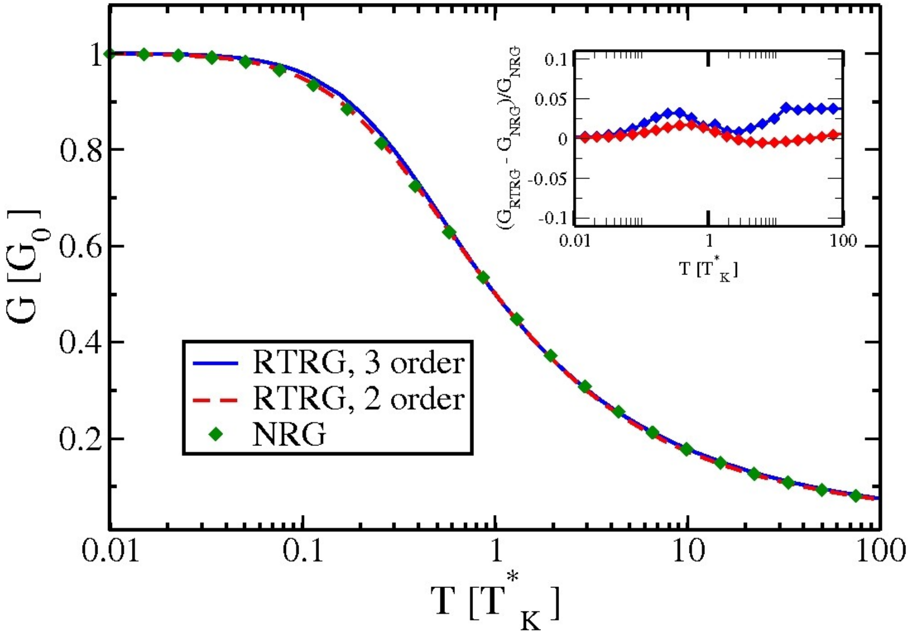
$$T, \frac{1}{t} \leq T_K = D e^{-1/(2J_0)}$$

time evolution



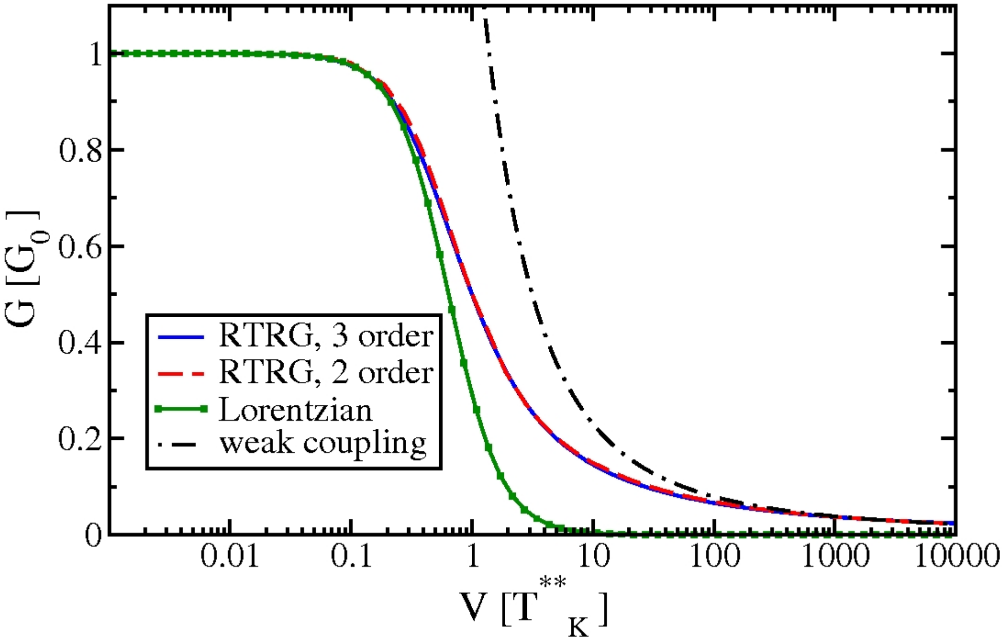
Stationary conductance G(T,V):

V=0: *G(T)*



→ agreement with NRG

T=0: *G(V)*



→ approx. independent of truncation order

$$G(T = T^*_K) \;=\; \frac{1}{2} G_0$$

$$\frac{T^*_K}{T^{**}_K} \approx 0.62$$

$$G(V = T^{**}_K) \;=\; \frac{1}{2} G_0$$

Fermi liquid coefficients : $T, V \ll T_K^*$

$$\frac{G(T,V)}{G_0} = 1 - c_T^* \left(\frac{T}{T_K^*}\right)^2 - c_V^* \left(\frac{V}{T_K^*}\right)^2$$

$$\frac{c_V^*}{c_T^*} = \frac{3}{2\pi^2}$$

NRG :

Merker et al., PRB 87, 165132 (2013)

$c_T^* \approx 6.58$ => $c_V^* = 3/(2\pi^2)\; c_T^* \approx 1.00$

RTRG :

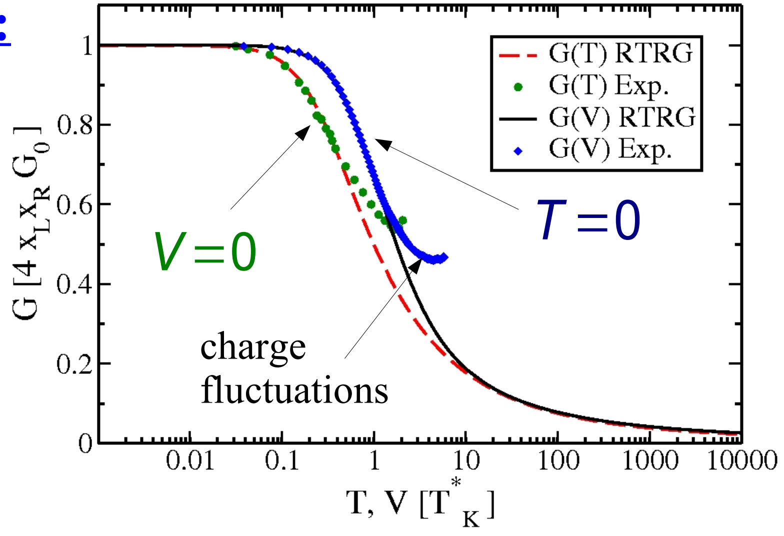
$c_T^* \approx 4.88$ 33% error

$c_V^* \approx 1.02$ 2% error

Stationary conductance: Comparison with experiment

Kretinin, Shtrikman & Mahalu,PRB 85, 201301(R) (2012)
Klochan, Micolich, Hamilton, Reuter, Wieck, Reininghaus, Pletyukhov & Schoeller, PRB 87, 201104(R) (2013)

T=0 or V=0 :



$$G(T=T^*_K) \;=\; \frac{1}{2}\,G_0$$

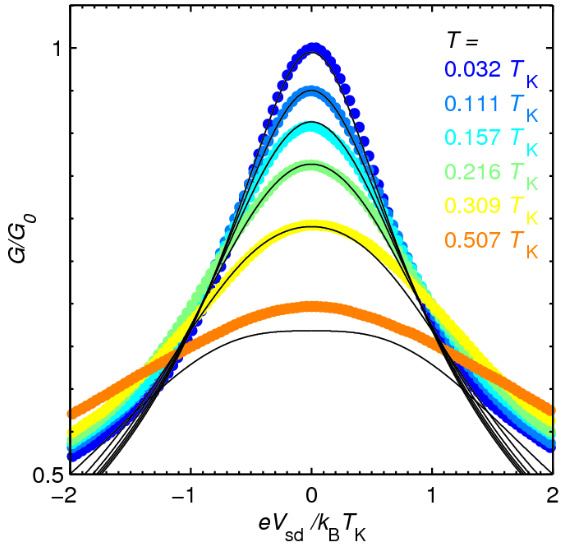
$$\boxed{G(V=T^*_K) \;=\; \frac{2}{3}\,G_0}$$

→ allows for an elegant exp. determination of T^*_K

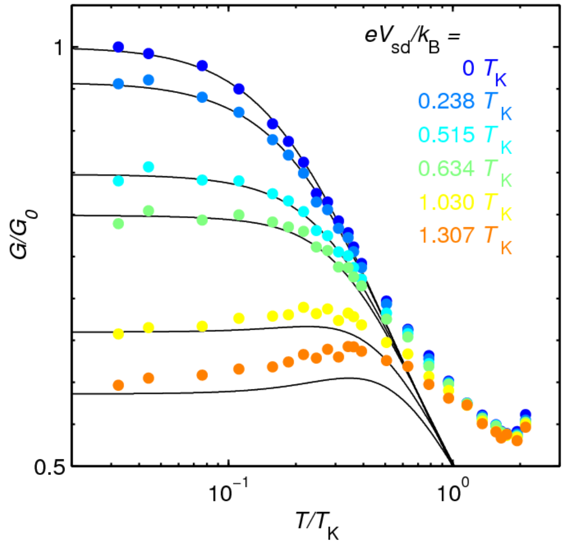
→ see also *Smirnov & Grifoni PRB 87, 121302(R) (2013)*

G(T,V) :

G(V) for different T

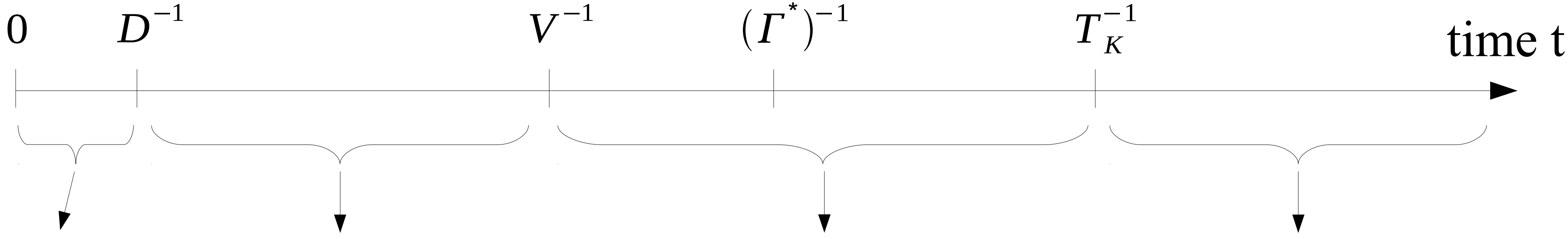


G(T) for different V



Spin dynamics at T=0 and large voltage $V \gg T_K$

$$D \gg V \gg \Gamma^* = \pi J_V^2 V \gg T_K \sim V e^{-\frac{1}{2 J_V}} \qquad J_V = \frac{1}{2\ln(V/T_K)}$$



non-universal

perturbative
in J_0

short times

sum up $(J_0 \ln(D t))^k$

$$\langle \underline{S} \rangle(t) = (1 - \frac{1}{|\ln(T_K t)|}) \langle \underline{S} \rangle(0)$$

long times

expand in $J_V \ln(V t) \ll 1$

$$\langle \underline{S} \rangle(t) = (1 - 2J_V - 2J_V^2 \ln(V t)) e^{-\Gamma^* t} \langle \underline{S} \rangle(0)$$
$$- \; 2J_V^2 \frac{1}{(V t)^2} \cos(V t) e^{-\Gamma^* t} \langle \underline{S} \rangle(0)$$

exponentially large times

$$J_V \ln(V t) \sim O(1)$$
$$J(E) \sim O(1)$$
$$\text{for } |E + nV + i\Gamma^*| \sim T_K$$

$$\langle \underline{S} \rangle(t) = ?$$

strong coupling problem!!

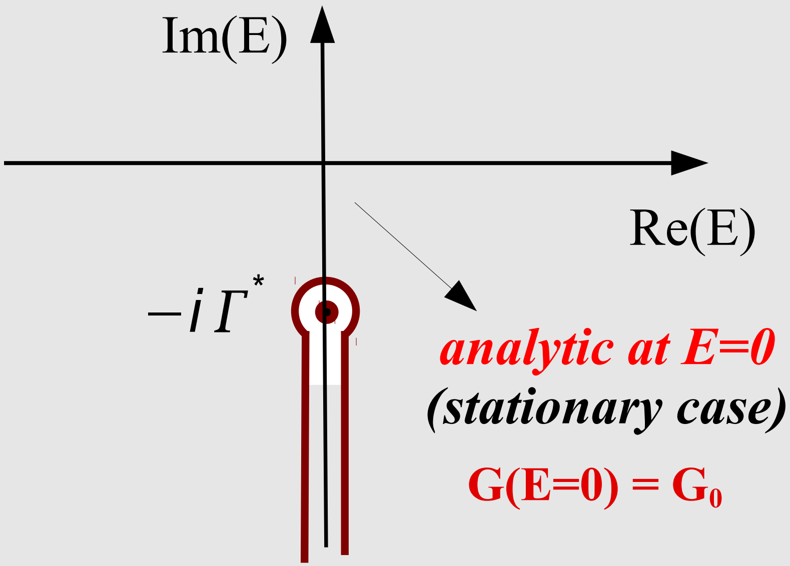
no cutoff by decay rates!!

Outlook: Spin dynamics in strong coupling

Long-time behaviour for T=h=V=0 :

N channels

N=1: Fermi liquid $\Gamma^* \sim T_K > 0$



analytic at E=0

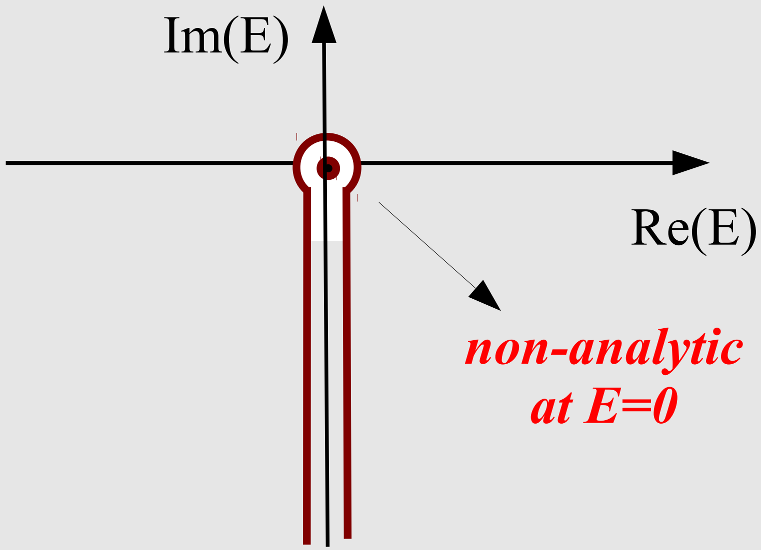
(stationary case)

G(E=0) = G_0

$$\langle \underline{S} \rangle(t) \;\sim\; (T_K t)^{-g} e^{-\Gamma^* t} \langle \underline{S} \rangle(0)$$

exponentiell + power law

N>1: non-Fermi liquid $\Gamma^* = 0$

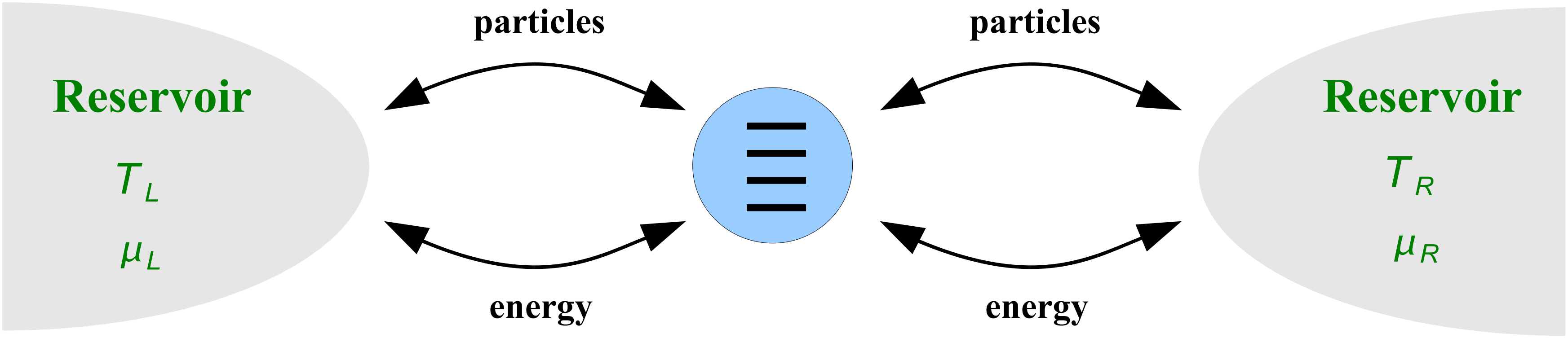


non-analytic at E=0

$$\langle \underline{S} \rangle(t) \;\sim\; (T_K t)^{-g} \langle \underline{S} \rangle(0)$$

pure power-law $\quad N \gg 1: \;\; g = \frac{4}{N}$

Summary



Real-time formalism is a useful tool at zero temperature :

- perturbative in effective system-reservoir coupling (fRG → perturbative in local Coulomb interaction)
- 1/E - divergencies → self-consistent perturbation theory
- logarithmic divergencies → renormalization group
- weak coupling → analytical solution possible
- strong coupling (e.g. Kondo) → useful but still open questions