Relaxation and Decoherence in Quantum Impurity Models: From Weak to Strong Tunneling

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- Quantum impurity models
  (spin-boson, Kondo, Schmid, BSG, ...)
- Dynamics
- From weak to strong tunneling
  - Quantum relaxation
  - Decoherence

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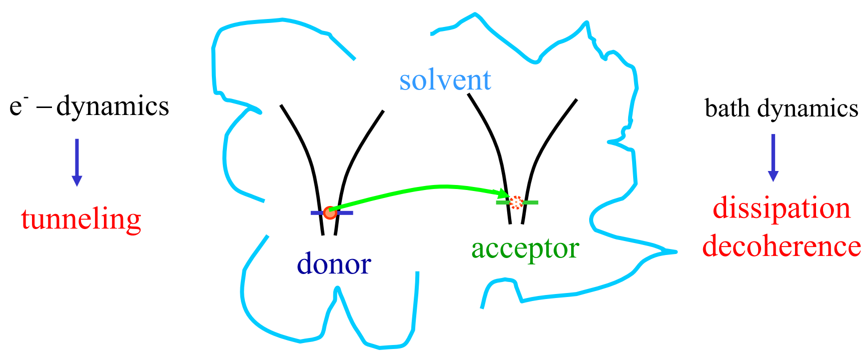
Electron transfer (ET):

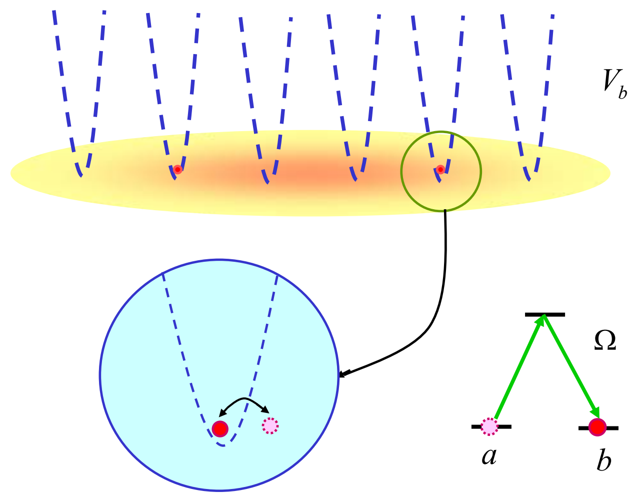


- biological electron transport
- molecular electronics
- quantum dots
- molecular wires
- charge transport in nanotubes

- classical rate theory
- Marcus theory of ET
  - activationless ET
  - inverted regime
- nonadiabatic ET
- adiabatic ET

Spin-boson model with ultracold atoms:

Recati *et al.* 2002



Global system:

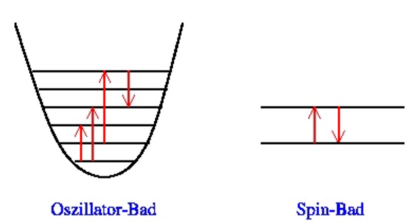
$$H = H_S + H_B + H_I$$

System

Heat bath T

Physical baths:

- Phonons
- Conduction electrons (Fermi liquid)
- 1d electrons (Luttinger liquid)
- BCS quasiparticles
- Electromagn env. (circuits, leads)
- Nuclear spins
- Solvent
- Electromagnetic modes

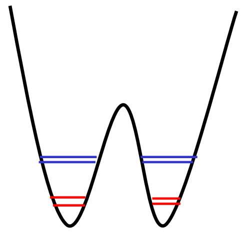


Spectral density of the coupling:

$$J(\omega \to 0) \propto \omega^s$$

s			
> 1	super-Ohmic	phonons $(d > 1)$
$= 1$	Ohmic	e-h excitations
< 1	sub-Ohmic	RC transmission line

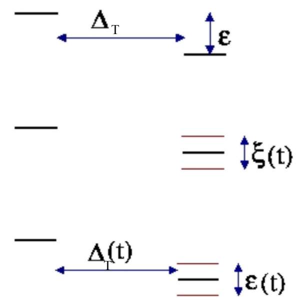
Truncated double well:



TSS:

stochastic force:

driven TSS:



Spin-boson Hamiltonian:

$$H = -\tfrac{1}{2}\Delta_T \sigma_x - \tfrac{1}{2}\varepsilon\,\sigma_z - \tfrac{1}{2}\underbrace{\sum\nolimits_\alpha c_\alpha x_\alpha(t)}_{\xi(t)}\,\sigma_z + \sum\nolimits_\alpha \left(\tfrac{p_\alpha^2}{2m_\alpha} + \tfrac{1}{2} m_\alpha\, \omega_\alpha^2\, x_\alpha^2\right)$$

$\langle \xi(t) \rangle_T = 0$ $\qquad \xi(t)$ stochastic force

$$\langle \xi(t)\xi(0)\rangle_T = \tfrac{1}{\pi}\int_0^\infty d\omega\, \mathrm{J}(\omega)[\coth(\omega/2T)\cos(\omega t) - i\sin(\omega t)]$$

Anisotropic Kondo model

$$H_K = \underbrace{v_F \sum_{k,\sigma} k c_{k,\sigma}^+ c_{k,\sigma}}_{\text{conduction band}} + \underbrace{\tfrac{1}{4} J_\parallel\, \tau_z \sum_\sigma \sigma\; c_\sigma^+ c_\sigma}_{\text{spin polarization conserved}} + \underbrace{\tfrac{1}{2} J_\perp (\tau_+ c_\downarrow^+ c_\uparrow + \tau_- c_\uparrow^+ c_\downarrow)}_{\text{spin flip scattering}}$$

Correspondence with spin-boson model:

$$\frac{\Delta_T}{\omega_c} \equiv \rho J_\perp \cos^2(\delta_K)$$

$$K \equiv (1 - 2\delta_K/\pi)^2$$

$$\delta_K(J_\parallel) \equiv \arctan(\pi\rho J_\parallel/4)$$

universal in the regime

$\rho J_\perp = \Delta/\omega_c << 1; \qquad |\rho J_\parallel| = |1-K| << 1$

ferromagnetic Kondo regime $J_\parallel < 0 \quad (K > 1)$

antiferromagn. Kondo regime $J_\parallel > 0 \quad (K < 1)$

Schmid model: particle in a tilted cosine potential

TB limit
$$H_S = -\tfrac{1}{2}\Delta_S \sum_n (a_n^* a_{n+1} + \text{h.c.}) - \tfrac{1}{2}[\,\varepsilon + \xi(t)\,] \sum_n n\, a_n^* a_n$$

- ❖ Current-biased Josephson junction (charge-phase duality)
- ❖ Impurity scattering in 1d quantum wire
- ❖ Point contact tunneling between quantum Hall edges

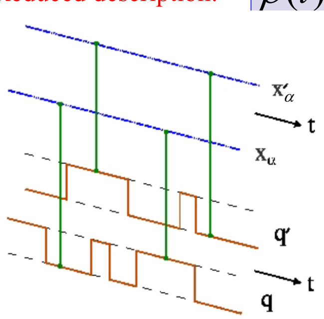
- ➢ Boundary sine-Gordon model
- ➢ Exact selfduality in the Ohmic scaling limit
- ➢ Scaling function for transport and noise at T=0 is known in analytic form

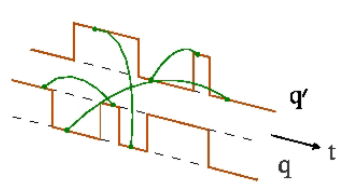
A. Schmid, Phys. Rev. Lett. 51, 1506 (1983)
P.Fendley, A.W.W. Ludwig, and H. Saleur, Phys. Rev. B 52, 8934 (1995)

Density matrix:

Global system: $W(t) = \sum_k p_k \,|\psi_k(t)\rangle\langle\psi_k(t)|$

Reduced description: $\rho(t) = \text{tr}_B\, W(t)$ partial trace





full dynamics: $W(t)$

time-local interactions

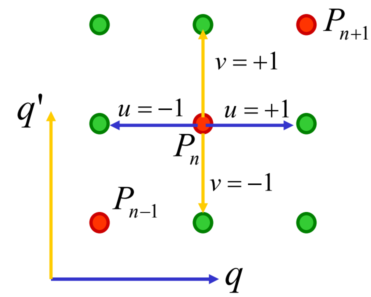
reduced dynamics: $\rho(t)$

time-nonlocal interactions

Tight-binding model:

charges $\{u_j = \pm 1\}$ $\{v_j = \pm 1\}$

$P_{0\to n}(t)$: $\sum_i u_i = n;$ $\sum_j v_j = n$



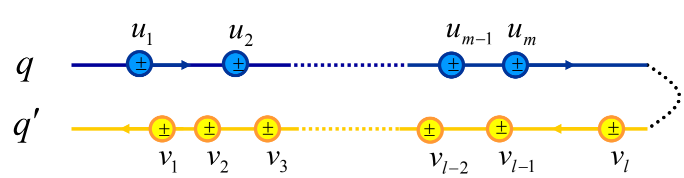
Influence functional:

$$\mathcal{F}[q_m, q'_l] = \exp\left\{ \sum_{j=2}^{m}\sum_{i=1}^{j-1} u_j u_i Q(t_j - t_i) + \sum_{j=2}^{l}\sum_{i=1}^{j-1} v_j v_i Q^*(t'_j - t'_i) - \sum_{j=1}^{l}\sum_{i=1}^{m} v_j u_i Q(t'_j - t_i) \right\}$$

Absorption and emission of energy according to detailed balance

$$Q(t - i/T) = Q^*(t)$$

Keldysh contour



$\sum_j u_j = \pm n;$ $\sum_i v_i = \pm n$

Laplace representation in the limit $\lambda \to 0$:

irreducible cluster $\equiv$ rate contribution $\gamma_{n,\alpha}^{(\pm)}$

Ohmic scaling limit:

Spectral density: $J(\omega) = 2\pi K \omega \qquad \omega < \omega_c$

Pair interaction between tunneling transitions:

$$Q(t) \equiv Q'(t) + iQ''(t) = 2K\left\{ \ln\left[\frac{\omega_c}{T\pi} \sinh(\pi T t) \right] + i\frac{\pi}{2}\mathrm{sgn}(t) \right\}$$

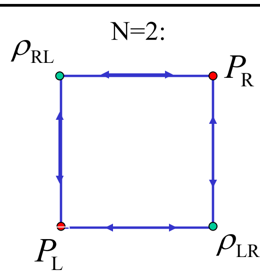
$$\xrightarrow{T=0} 2K \ln(\omega_c t) + i\pi K\, \mathrm{sgn}(t)]$$

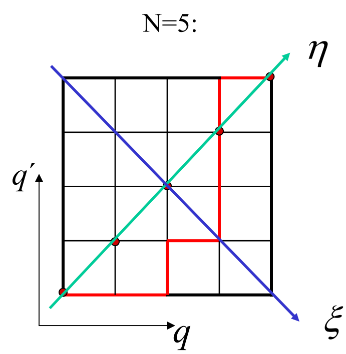
Kondo scale:

$$\varepsilon_K = \left(\frac{\Gamma(1-K)}{2^K} \right)^{\frac{1}{1-K}} \left(\frac{\Delta_T}{\omega_c} \right)^{\frac{K}{1-K}} \Delta_T \qquad \text{TSS model}$$

$$\varepsilon_K = 2\left(\frac{\pi}{\Gamma(K)} \right)^{\frac{1}{1-K}} \left(\frac{\Delta_S}{\omega_c} \right)^{\frac{K}{1-K}} \Delta_S \qquad \text{Schmid model}$$

at fixed Kondo scale $\Delta_T = 2\sin(\pi K)\Delta_S$





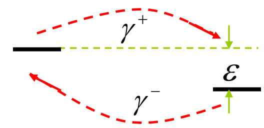
charges: $\xi_j = \pm 1; \quad p_j = \sum_{k=1}^{j} \xi_k; \quad \eta_j = \pm 1$

scaling limit: $\mathcal{F}_{2m} = \exp[i\pi K \sum_{j=1}^{2m-1} p_j \eta_j] \times \exp[\sum_{j=2}^{2m} \sum_{k=1}^{j-1} \xi_j \xi_k Q''(t_j - t_k)]$

friction ⇩ phase factor

noise (Gaussian filter) ⇩ noise integral

Incoherent tunneling:



golden rule limit: $\gamma^{\pm} = \frac{\pi}{2}\Delta^2\, p(\pm\varepsilon)$

$p(\pm\varepsilon)$ is probability for transfer of energy $\varepsilon \left\{ \begin{matrix} \text{to} \\ \text{from} \end{matrix} \right\}$ the bath

$$p(\pm\varepsilon) = \cos(\pi K)\,\tfrac{1}{\pi}\int_0^\infty \mathrm{d}t\ \cos(\varepsilon\, t)\, e^{-Q''(t)} \pm \sin(\pi K)\,\tfrac{1}{\pi}\int_0^\infty \mathrm{d}t\, \sin(\varepsilon t)\, \mathrm{e}^{-Q''(t)}$$

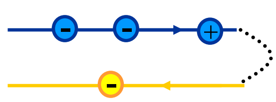
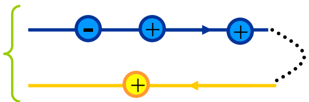
phase factor noise integral phase factor noise integral

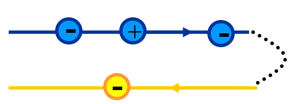
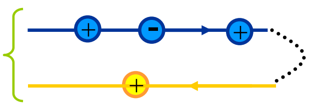
$\varepsilon = 0$: $$\gamma^+ = \gamma^- = \frac{\sqrt{\pi}\,\Gamma(K)}{4\Gamma(K+\frac{1}{2})}\frac{\Delta^2}{\omega_c}\left(\frac{\pi T}{\omega_c}\right)^{2K-1}$$

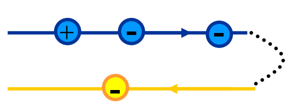
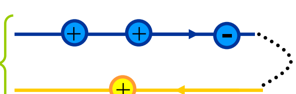
$T = 0$: $$\gamma^+ = \frac{\pi}{2\Gamma(2\mathrm{K})}\frac{\Delta^2}{\omega_c}\left(\frac{\varepsilon}{\omega_c}\right)^{2K-1} \quad ; \qquad \gamma^- = 0\,;$$

Order Δ^4:

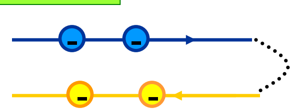
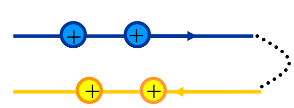
$\gamma_1^{(\pm)}$: $\gamma_1^{(-)} = \mathrm{e}^{-\varepsilon/T}\,\gamma_1^{(+)}$

(1)  $+\ \text{c.c.} = \mathrm{e}^{-\varepsilon/T}\Big\{$  $+\ \text{c.c.}\Big\}$

(2)  $+\ \text{c.c.} = \mathrm{e}^{-\varepsilon/T}\Big\{$  $+\ \text{c.c.}\Big\}$

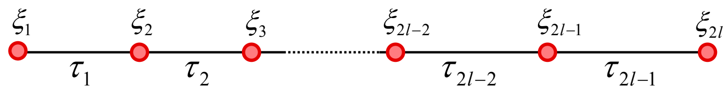
(3)  $+\ \text{c.c.} = \mathrm{e}^{-\varepsilon/T}\Big\{$  $+\ \text{c.c.}\Big\}$

$\gamma_2^{(\pm)}$: $\gamma_2^{(-)} = \mathrm{e}^{-2\varepsilon/T}\,\gamma_2^{(+)}$

(4)  $= \mathrm{e}^{-2\varepsilon/T}$ 

Noise integrals:

$T = 0$



$$I_l^{\pm}(\vec{\xi}) = \int_0^{\infty} \mathcal{D}_{2l-1}(\vec{\tau}) \begin{Bmatrix} \cos\left(\varepsilon \sum_{j=1}^{2l-1} p_j \tau_j\right) \\ \sin\left(\varepsilon \sum_{j=1}^{2l-1} p_j \tau_j\right) \end{Bmatrix} \exp\left(2K \sum_{j>i=1}^{2l} \xi_j \xi_i \ln(\omega_c \tau_{ji}) \right)_{\text{irred}}$$

- Up-hill partial rates are zero $\gamma_{n,\alpha}^{-} = 0$ — general!
- Scaling property $I_l^{+}(\vec{\xi}) = \tan(\pi K l)\, I_l^{-}(\vec{\xi})$ if all p_j have same sign — particular!

Formidable relations between the various noise integrals of same order l

Results:

Schmid model:

- Only minimal number of transitions contribute to the rate $\gamma_n^{+} = O(\Delta^{2n})$

- All rates can be reconstructed from the known mobility $\mu \propto \sum_n n \gamma_n^{+}$
- Knowledge of all statistical fluctuations (full probability distribution)

H. Saleur and U.Weiss, Phys. Rev. B 63, 201302(R) (2001)

TSS model:

- Exact relations between rates of the Schmid and TSS model

$$\tilde{\gamma}_n^{+} = (-1)^{n-1} 4 \sin^2(n\pi K)\, \gamma_n^{+}$$

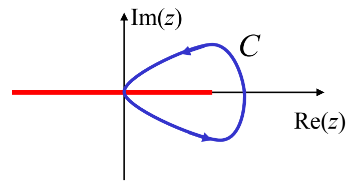
Weak-tunneling expansion

$\nu \equiv \varepsilon / \varepsilon_{\mathrm{K}}$

$$\tilde{\gamma}^{+} = \frac{\varepsilon}{2\sqrt{\pi}} \sum_{m=1}^{\infty} \frac{1}{m!} \frac{\Gamma(Km)[1-\cos(2\pi K m)]}{\Gamma[\frac{3}{2}+(K-1)m]} \nu^{(2K-2)m}$$

Integral representation

$$\tilde{\gamma}^{+} = \mathrm{Re}\, \frac{\varepsilon}{2\pi i} \int_C \frac{\mathrm{d}z}{z} \left[\sqrt{z-1-z^K \,\mathrm{e}^{i2\pi K}\, \nu^{2K-2}} - \sqrt{z-1-z^K \nu^{2K-2}} \right]$$



H. Baur, A. Fubini, and U.Weiss, cond-mat/0211046

Strong-tunneling expansion

$\nu \equiv \varepsilon / \varepsilon_{\mathrm{K}}$

The case K<1:

$$\tilde{\gamma}^{+} = \sum_{n=0}^{\infty} \tilde{\gamma}_n^{+} ; \qquad \tilde{\gamma}_n^{+} = \frac{\varepsilon}{2\sqrt{\pi}} b_n(K)\, \nu^{2n-1}$$

$\frac{1}{3} < K < 1$:

$$b_n(K) = d_n(K) \equiv \frac{1}{n!} \frac{\Gamma[(\frac{1}{2}-n)\frac{K}{1-K}]}{(\frac{1}{2}-n)\,\Gamma[(\frac{1}{2}-n)\frac{1}{1-K}]}$$

$K \le \frac{1}{3}$:

$$b_n(K) = 2\sin^2[\tfrac{\pi K}{1-K}(\tfrac{1}{2}-n)]\, d_n(K)$$

Leading asymptotic term:

$\varepsilon \to 0$:

$$\tilde{\gamma}_0^{+} = \tfrac{1}{2\sqrt{\pi}} b_0(K)\, \varepsilon_{\mathrm{K}}$$

Strong-tunneling expansion

$$\nu \equiv \varepsilon / \varepsilon_{\mathrm{K}}$$

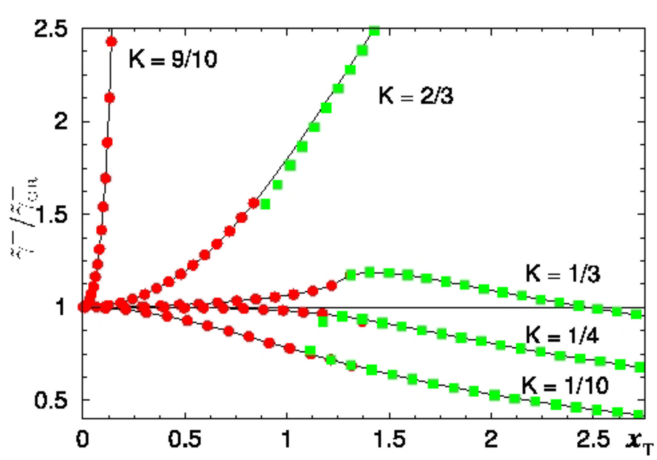
The case K>1:

$K = p + \kappa$
p integer
$0 \le \kappa < 1$

$$\tilde{\gamma}^{+} = \frac{\varepsilon}{2\sqrt{\pi}} \sum_{m=1}^{\infty} c_m(K)\, \nu^{(2/K-2)m}$$

$$c_m(K) = \frac{(-1)^m}{m!} \frac{2\Gamma(\frac{m}{K})\sin[\frac{1+p}{K} m\pi]\sin(\frac{p}{K} m\pi)}{K\,\Gamma[\frac{3}{2}+(\frac{1}{K}-1)m]}$$

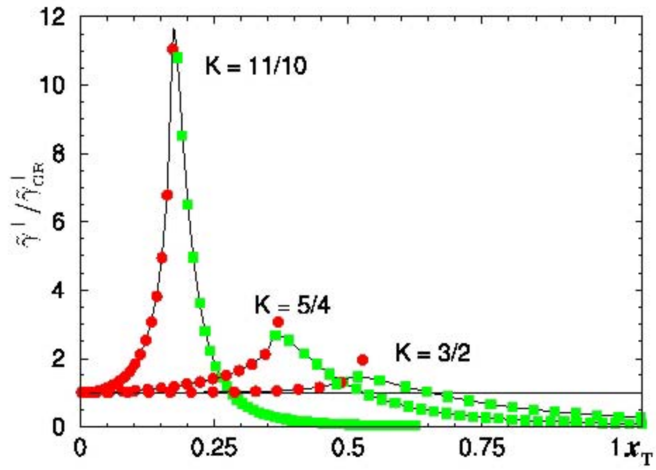
$0 < K < 1$



weak tunneling
large bias

strong tunneling
small bias

$K > 1$



weak tunneling
small bias

strong tunneling
large bias

Decoherence

$K < \frac{1}{2}$

$$\gamma^{\mathrm{dec}} = \sum_{n=0}^{\infty} \gamma_n^{\mathrm{dec}}$$

Conjecture: holds in all known special cases

$$\frac{\gamma_n^{\mathrm{dec}}}{\tilde{\gamma}_{\mathrm{n}}^{+}} = \begin{cases} \frac{1}{2} & K \le \frac{1}{3} \\ \sin^2\left[\frac{\pi K}{1-K}\left(\frac{1}{2}-n\right)\right] & \frac{1}{3} < K < \frac{1}{2} \end{cases}$$

Strong-tunneling expansion:

$$\gamma^{\mathrm{dec}} = \frac{\varepsilon}{2\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\Gamma\left[\left(\frac{1}{2}-n\right)\frac{K}{1-K}\right]}{\left(\frac{1}{2}-n\right)\Gamma\left[\left(\frac{1}{2}-n\right)\frac{1}{1-K}\right]} \sin^2\left[\frac{\pi K}{1-K}\left(\frac{1}{2}-n\right)\right] v^{2n-1}$$