Real-time dynamics in Quantum Impurity Systems: A Time-dependent Numerical Renormalization Group Approach

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Concepts in Electron Correlation, Hvar, 30. September 2005

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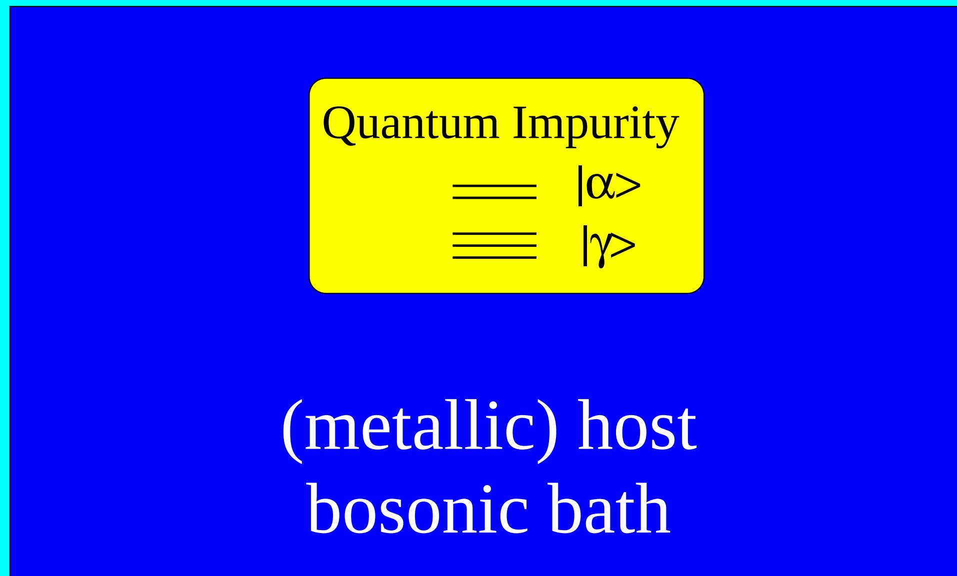
What is a Quantum-Impurity System (QIS)?



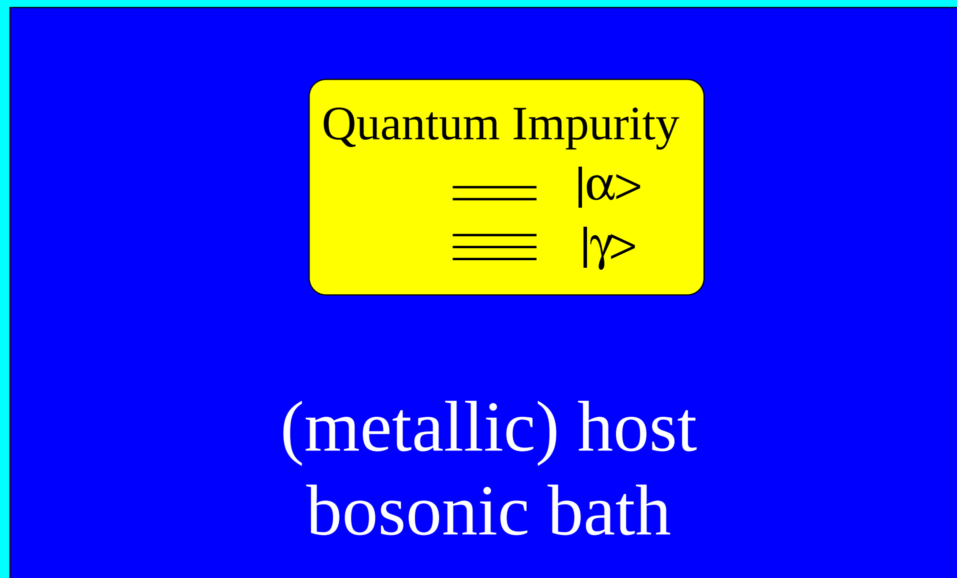
quantum-impurity:

- embedded in a (metallic) host
- interacting with the environment of non-interacting particles (Bosons/Fermions)

Problem:

- infrared divergence due to local degeneracy

What is a Quantum-Impurity System (QIS)?



Examples:

- transition metal ion Cu, Mn, Ce in a metal
- two-level system (Qubit) in a bosonic bath
- Quantum dot coupled to leads
- donor-acceptor centers of a large bio-molecule
- . . .

Goal of the Talk

Our new Approach to Non-Equilibrium of QIS:

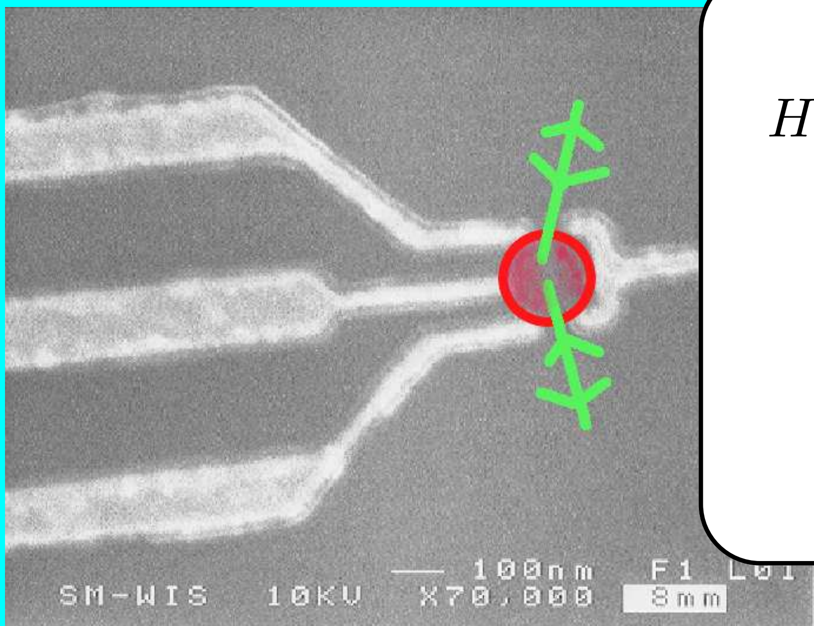
- based on the non-perturbative NRG
- uses the *complete basis of the many body Fock space*
- takes into account *all energy scales*
- describes short and long time scales
- does not accummulate an error $\propto t$ as the TD-DMRG

☞ breakthrough in the description of real time dynamics of non-equilibrium quantum systems:

Contents

1. Introduction
   - Modelling of quantum dots
   - Charge transfer in molecules (spin-boson model)
2. Non-equilibrium dynamics
   - Time evolution of quantum systems
   - New approach to quantum impurity problems
3. Results
   - Dissipation and decoherence in a two level system
   - Spin- and charge dynamics in ulta-small quantum dots
   - AF-Kondo model
     - spin precession
4. Summary and outlook

Modelling of a Quantum Dot



$$H = \sum_{k\sigma} \epsilon_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma} + \sum_{\sigma} \left[E_d(t) - \sigma H(t)\right] d^\dagger_\sigma d_\sigma + U n^d_\uparrow n^d_\downarrow + \sum_{k\sigma} V(t) \left(c^\dagger_{k\sigma} d_\sigma + d^\dagger_\sigma c_{k\sigma} \right)$$

Single Impurity Anderson Model (SIAM)

- charge fluctuation scale: $\Gamma_i = V_i^2 \pi \rho_F$
- infrared problem
  ☞ low temperature scale: $T_K \propto \exp(-\pi U / 8\Gamma)$

Spin-Boson Model

- qubit plus environment (Unruh)
- electron transfer in (bio)-molecules (Marcus, Schulten)

$$|\uparrow\rangle = |A\rangle, \; |\downarrow\rangle = |D\rangle$$

$$H = \epsilon\sigma_z - \frac{\Delta}{2}\sigma_x + \sum_q \hbar\omega_q b_q^\dagger b_q + \sigma_z \sum_q M_q \left(b_q^\dagger + b_q\right)$$

$$J(\omega) = \sum_q |M_q|^2 \delta(\omega - \omega_q) \propto 2\pi\alpha\omega_c^{1-s}\omega^s$$

Leggett *et. al.* (RMP 1987), Xu and Schulten 1994, Bulla *et. al.* (2003) $\cdots$

Questions:

- influence of the bosonic spectrum $J(\omega)$ on the real time dynamics
- critical slowdown of the charge transfer process for large coupling

Where do we stand in the

description of non-equilibrium,

dissipation and decoherence

in quantum systems?

Non-Equilibrium Dynamics of Quantum Systems

quantum dynamics

- single quantum state: Schrödinger equation

$$i\hbar\partial_t|\psi >= H(t)|\psi >$$

- ensemble: density operator

$$i\hbar\, \partial_t \hat{\rho}(t) = [H, \hat{\rho}] \quad ; \quad \rho(t) = e^{-iHt/\hbar}\rho_0 e^{iHt/\hbar}$$

finite size quantum system: only unitary dynamics, no dissipation

dissipation and decoherence:
infinitly large environment needed

$$\frac{\text{Size of Subsystem}}{\text{Size of environment}} \longrightarrow 0$$

Subsystem

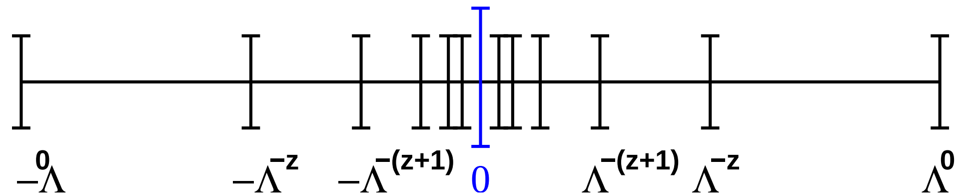
Environment

NRG Approach to Quantum Impurity Problems

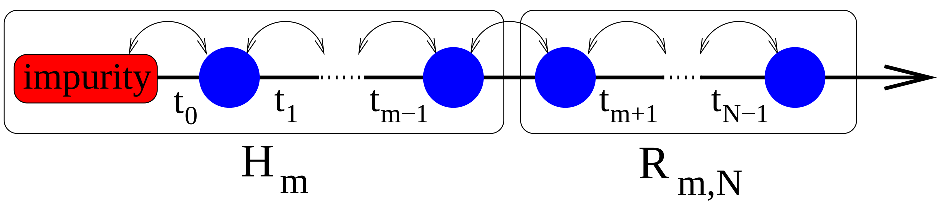
$$H = H_{imp} + H_{bath} + H_{imp-bath}$$

1. discretizing the bath Hamiltonian on a logarithmic energy mesh

   (Wilson 1975,Oliveira)



2. mapping onto a semi-infinite chain

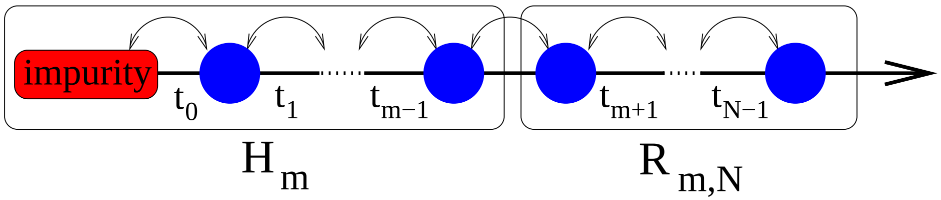


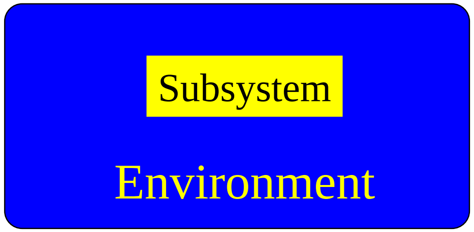
3. diagonalizing the Hamiltonian H_{N+1} using the recursion

$$H_{N+1} = \sqrt{\Lambda} H_N + \sum_{\alpha} \xi_{N\alpha} \left(f^\dagger_{N+1\alpha} f_{N\alpha} + f^\dagger_{N\alpha} f_{N+1\alpha} \right)$$

4. truncate the basis set, go back to step 3

Novel Many-Body Approach to NEQ of QIS





- use the NRG to generate a complete basis $|l, e; m\rangle$
  - $H_m|l\rangle = E_l^m|l\rangle$, l eliminated state
  - $e \in R_{m,N}$

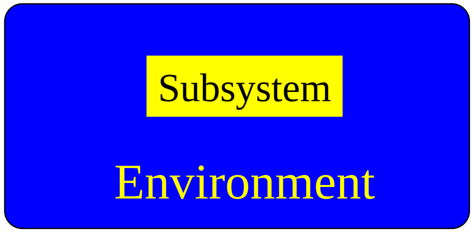
$$1 = \sum_m \sum_{l,e} |l, e; m\rangle\langle l, e; m|$$

- Puls at $t = 0$: $H(t) = H_i\Theta(-t) + H_f\Theta(t)$
- operator $\hat{O}$: property of the subsystem S

Novel Many-Body Approach to NEQ of QIS

time-dependent NRG (TD-NRG)

(FBA, A. Schiller, cond-mat/0505553, PRL 2005)



- calculate $\rho^{red}_{NEQ}(t)$

$$\langle \hat{O} \rangle (t) = \mathrm{Tr}\left[\rho(t)\hat{O}\right] = \sum_{m,\alpha\alpha'} \langle \alpha | \hat{O} | \alpha' \rangle \rho^{red}_{\alpha\alpha',m}(t)$$

$$\rho^{red}_{\alpha\alpha',m}(t) = e^{-i(E_\alpha - E_{\alpha'})t} \sum_{e} \langle \alpha, e; m | \rho_{eq} | \alpha', e; m \rangle$$

Feynman 1972, White 1992, Hofstetter 2000, $\cdots$

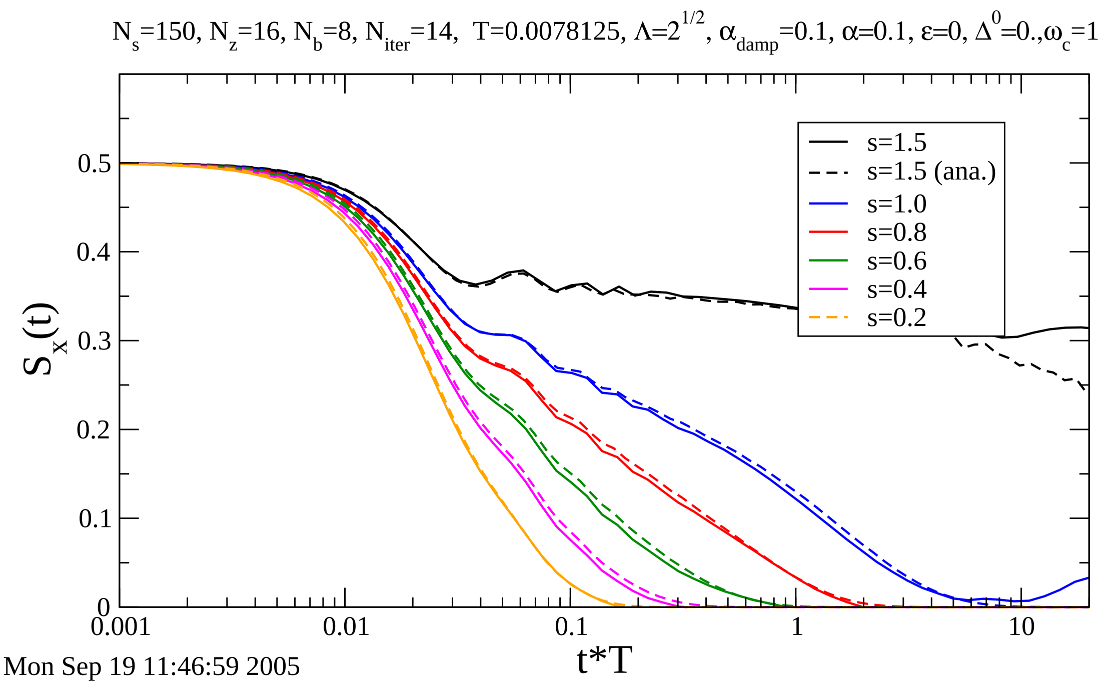
- mimic bath contiuum: use Oliveira's z-trick
- evolves towards the new steady state: $[H(t>0), \rho(\infty)] = 0$

Trace over the environment: dissipation and decoherence!

Spin-Boson Model

$$H = \epsilon\sigma_z - \frac{\Delta}{2}\sigma_x + \sum_q \hbar\omega_q b_q^\dagger b_q + \sigma_z \sum_q M_q\left(b_q^\dagger + b_q\right)$$

$$S_x = \frac{1}{2}\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right)$$



Decoherence

- QuBit state

$$\frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$$

- exact solution

$$P(t) = e^{-\Gamma(t)}$$

Leggett *et al.*, Unruh, Palma *et al.* , Bulla *et al.*

Spin-Boson Model

$$H = \epsilon\sigma_z - \frac{\Delta}{2}\sigma_x + \sum_q \hbar\omega_q b_q^\dagger b_q + \sigma_z \sum_q M_q \left(b_q^\dagger + b_q\right)$$

$J(\omega) = 2\pi\alpha\omega_c^{1-s}\omega^s$ for $0 < \omega < \omega_c$; Ohmic case: $s = 1$

Fixed point: delocalized

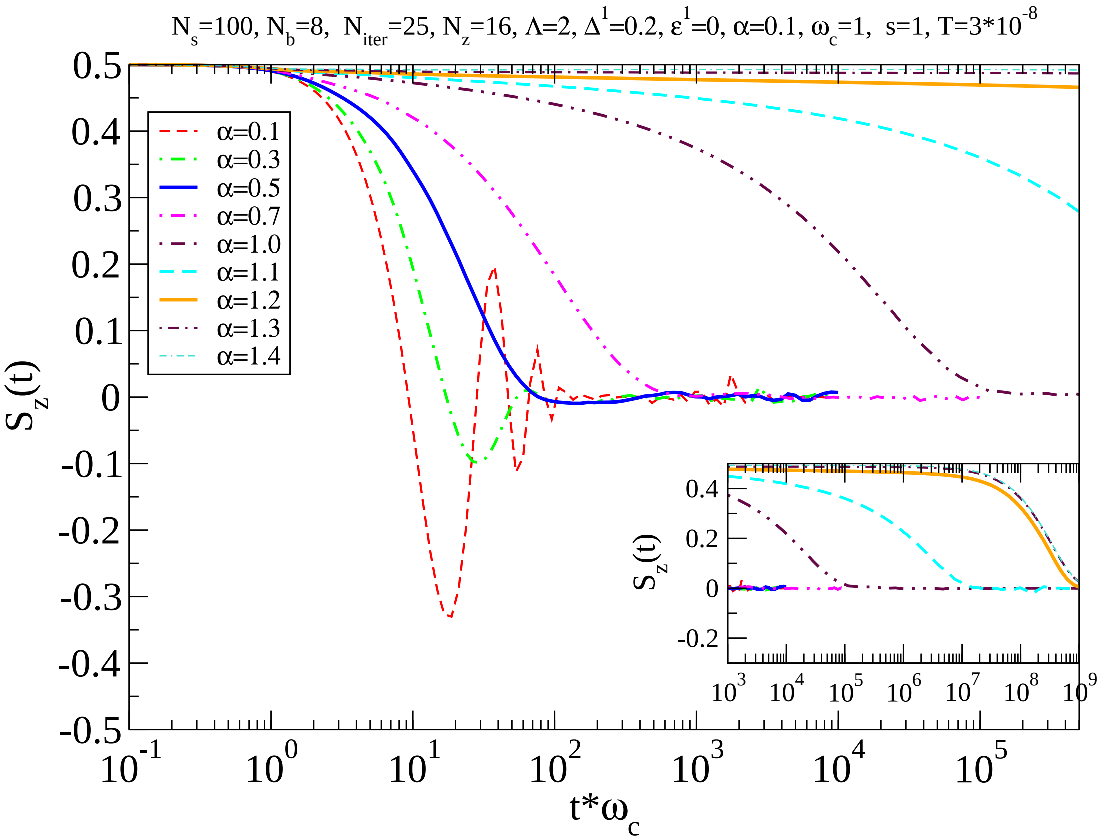
$0<\alpha<1/2$	Toulouse Point: $\alpha=1/2$	$1/2<\alpha<\alpha_c(\Delta)$
oszillatory		overdamped

localized

$\alpha_c(\Delta) < \alpha$

Spin-Boson Model

$$H = \epsilon\sigma_z - \frac{\Delta}{2}\sigma_x + \sum_q \hbar\omega_q b_q^\dagger b_q + \sigma_z \sum_q M_q \left(b_q^\dagger + b_q\right)$$

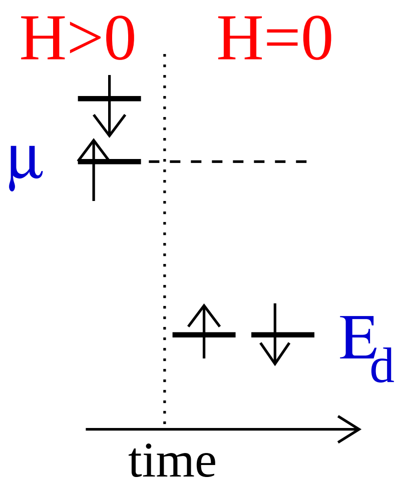


$$J(\omega) \quad = \quad 2\pi\alpha\omega_c^{1-s}\omega^s$$

Ohmic Regime: $s = 1$

- QPT at $\alpha_c(\Delta)$
- Toulouse point $\alpha = 1/2$
- oszillatory $\alpha < 1/2$
  overdamped $\alpha_c > \alpha > 1/2$
- localize: $\alpha > \alpha_c$

Charge Fluctuation in a Small Quantum Dot

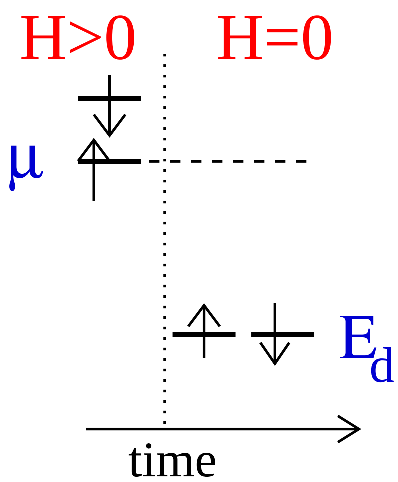


impurity levels

$$H = \sum_{k\sigma} \epsilon_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma} + \sum_{\sigma} \left[E_d(t) - \sigma H(t)\right] d^\dagger_\sigma d_\sigma + U n^d_\uparrow n^d_\downarrow + \sum_{k\sigma} V(t) \left(c^\dagger_{k\sigma} d_\sigma + d^\dagger_\sigma c_{k\sigma} \right)$$

- change of E_d: change dynamics
- change of mag. field H: spin dynamics
- change of V: route to new equilibrium

Charge Fluctuation in a Small Quantum Dot



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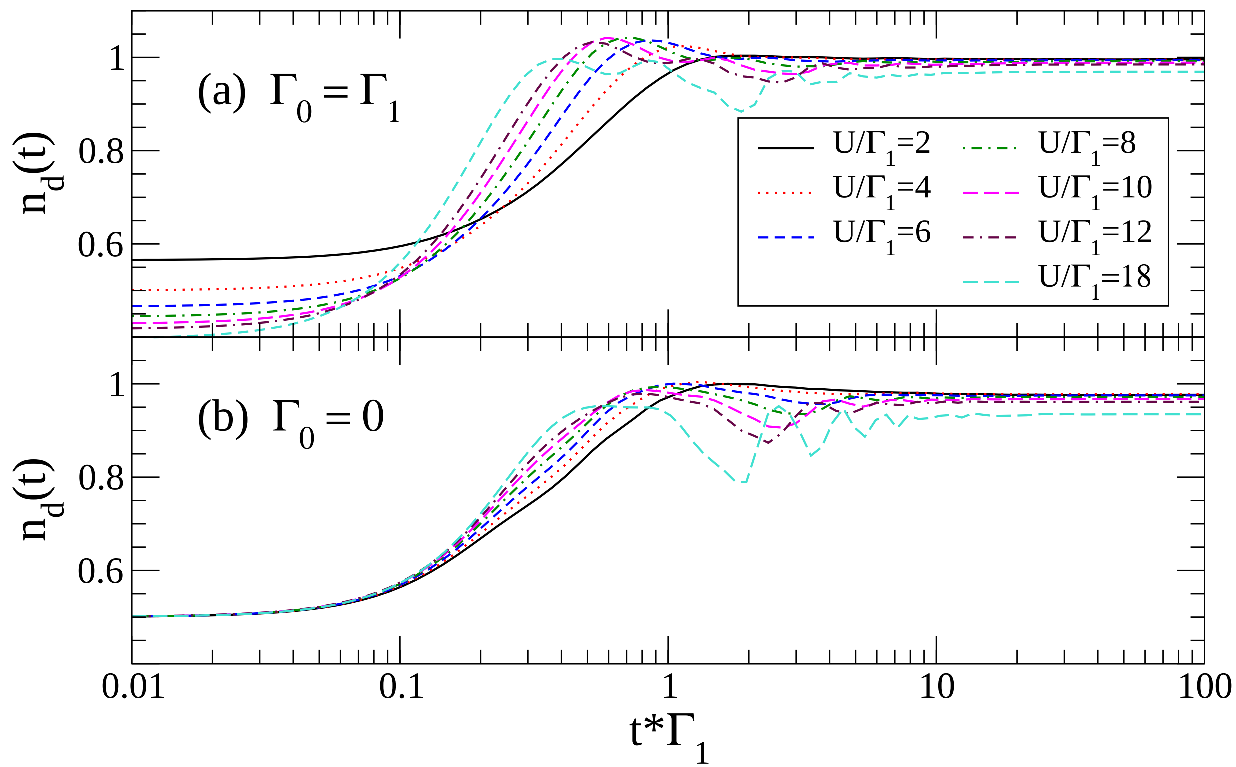
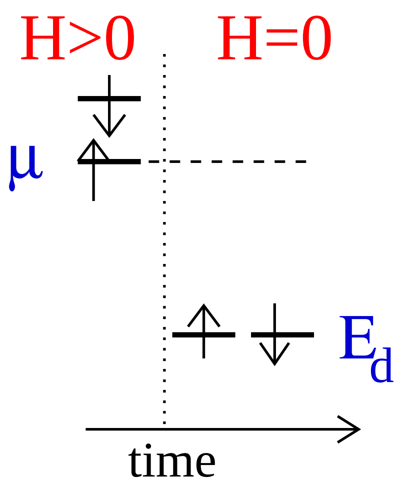
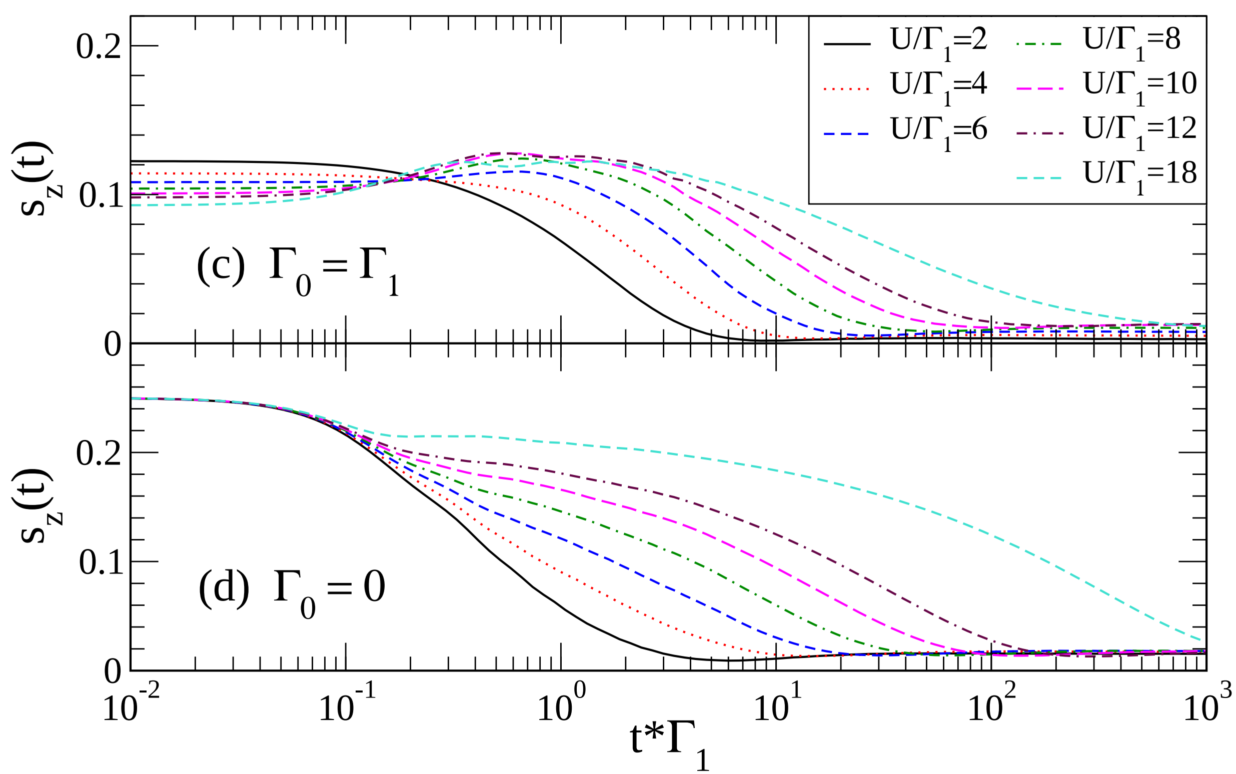


Charge relaxation time scale : $t_{ch} = 1/\Gamma_1$

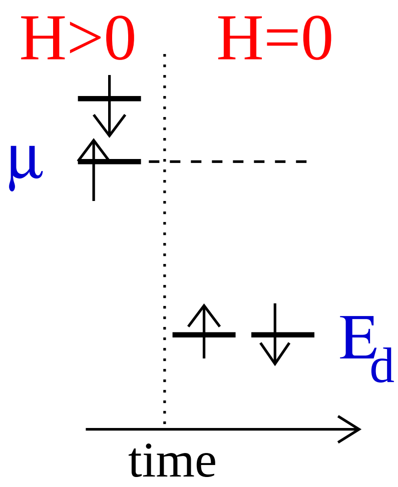
Spin Fluctuation in a Small Quantum Dot



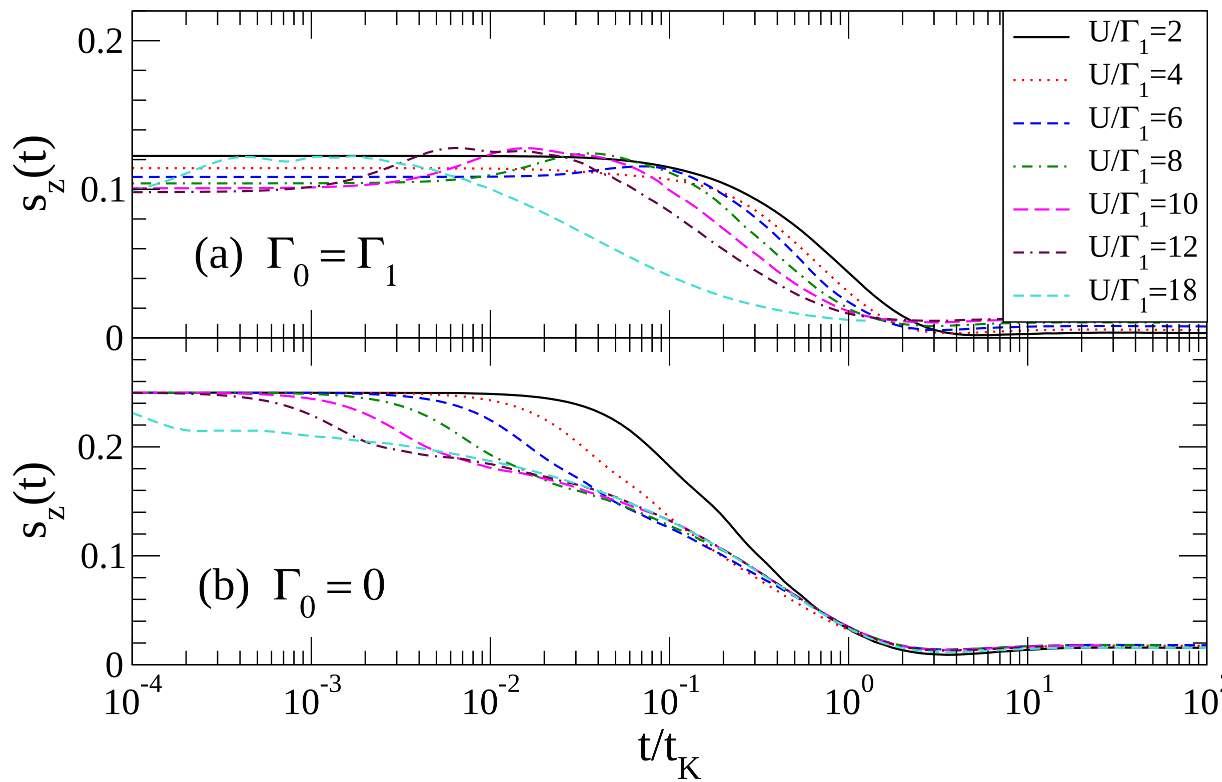
impurity levels



Spin Fluctuation in a Small Quantum Dot

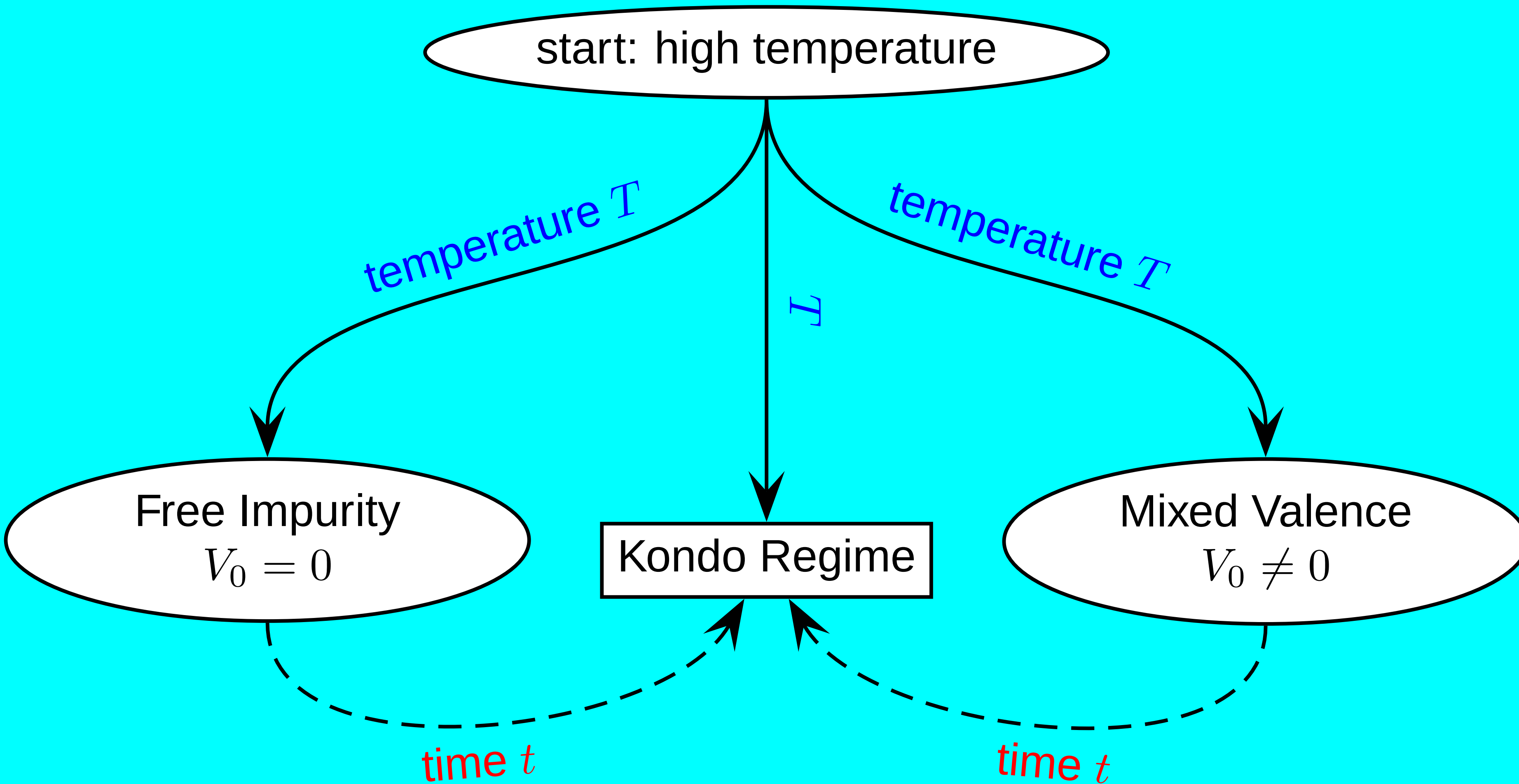


impurity levels



Spin relaxation time scale : $t_{sp} \propto 1/T_K$

SIAM Time-Evolution

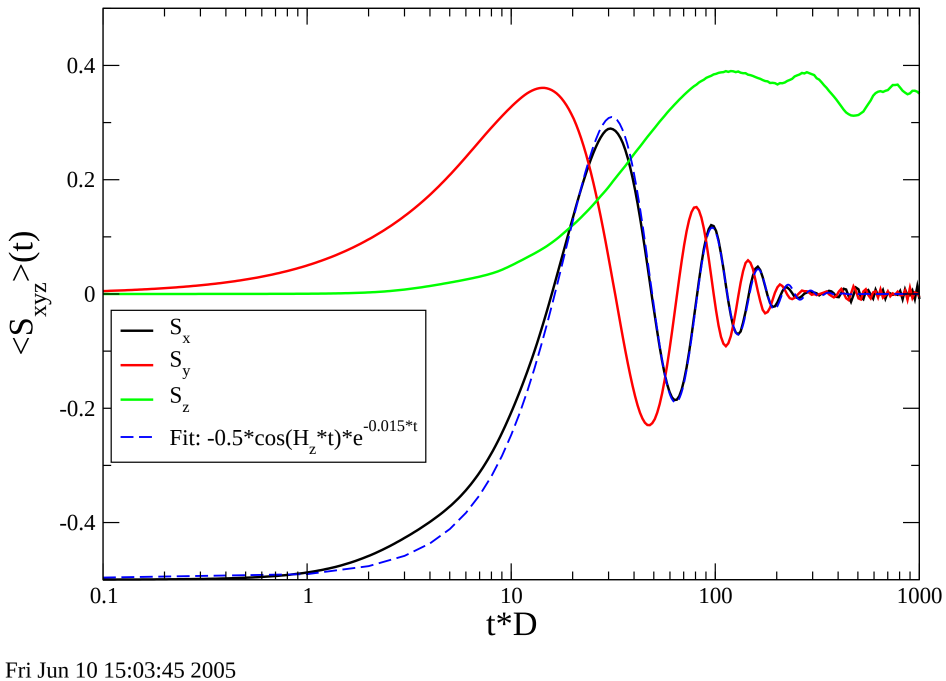


- no universality
- time evolution depends on boundary conditions

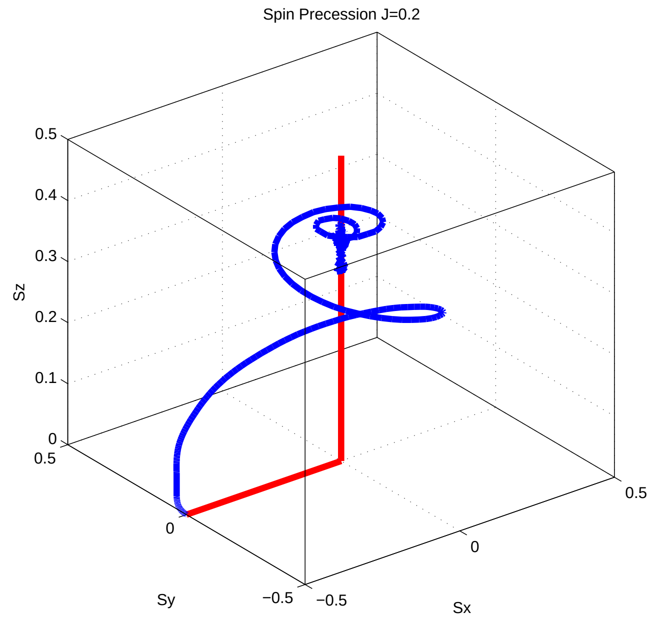
Kondo Model

$$H = H_{cb} + \frac{H_z(t)}{2}\sigma_z + \frac{H_x(t)}{2}\sigma_x + J\vec{S}_{loc} \cdot \vec{s}_{cb}$$

Spin Precession: $H_x = 0.1 \rightarrow H_z$



external magnetic field: $x \rightarrow z$-axis



Summary and Outlook

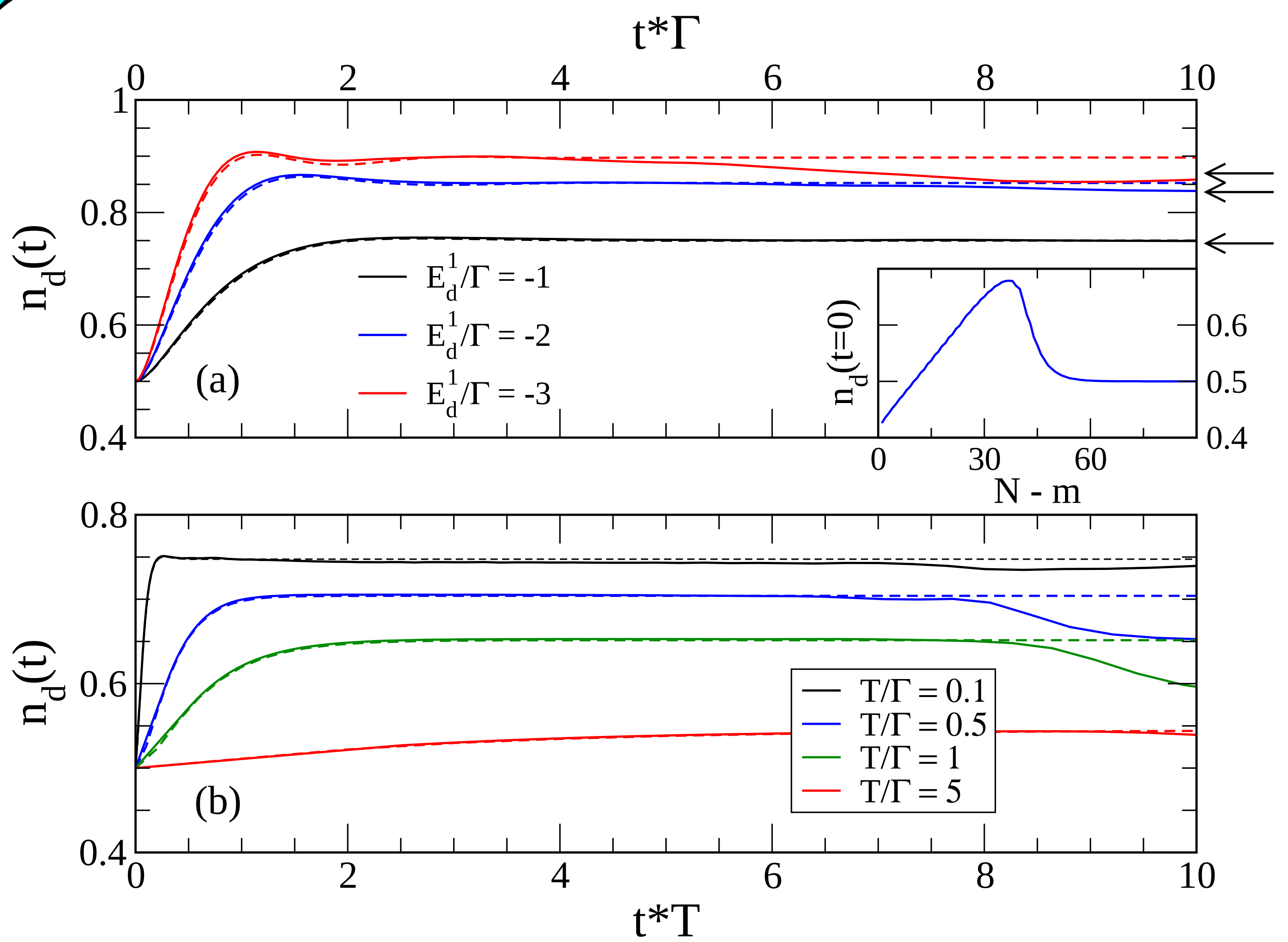
TD-NRG algorithm:

- complete basis set needed for the time evolution
- dissipation and decoherence due to the bath
- Spin-Boson Model
  - benchmark: decoherence and non-ohmic baths
  - oscillatory vs overdamped regime
- SIAM:
  - two relaxation time scale for spin and charge dynamics
- Kondo Model:
  - spin relaxation and spin precession

Outlook

- Bosonic QI models: charge transfer in bio-molecules, photosynthesis
- description of steady state currents

Benchmark: Resonant Level Model



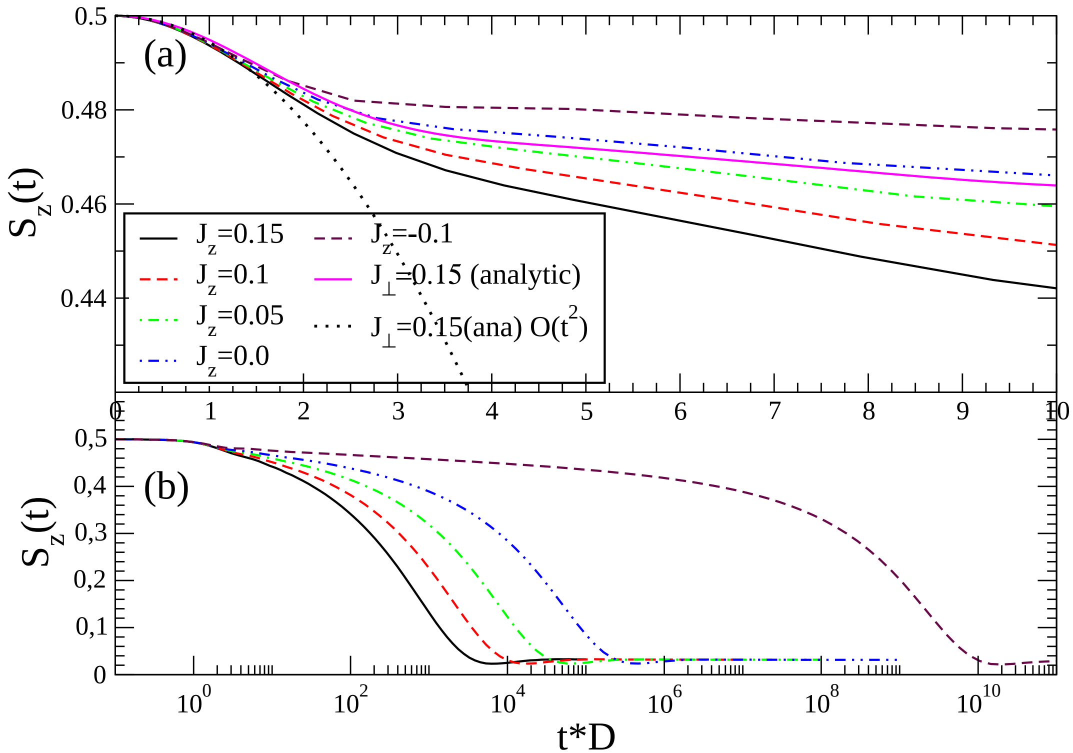
Anisotropic Kondo Model

$$H = H_{cb} + \frac{H_z(t)}{2}\sigma_z + \frac{H_x(t)}{2}\sigma_x + \sum_{kk'\alpha\beta} \frac{J_z(t)}{2} c^\dagger_{k\alpha} c^\dagger_{k'\beta} \sigma_z S^z_{imp}$$

$$+ \sum_{kk'} \frac{J_{perp}(t)}{2} \left(c^\dagger_{k\uparrow} c^\dagger_{k'\downarrow} S^-_{imp} + c^\dagger_{k\downarrow} c^\dagger_{k'\uparrow} S^+_{imp} \right)$$

Anisotropic Kondo Model

spin relaxation: $J^0 = 0, J_\perp^1 = 0.15D = const$



two regimes:

- short time scale
  analytical result:

$$S_z(t) - S_z(0) \propto (2\rho J_\perp^1)^2$$
$$\times [G(2Dt) - 2G(Dt)]$$

$$G(x) = \sum_{l=1}^{\infty} \frac{(-1)^{l+1}}{(2l)!2l(2l-1)} x^{2l}$$

external magnetic field: z-axis

Anisotropic Kondo Model

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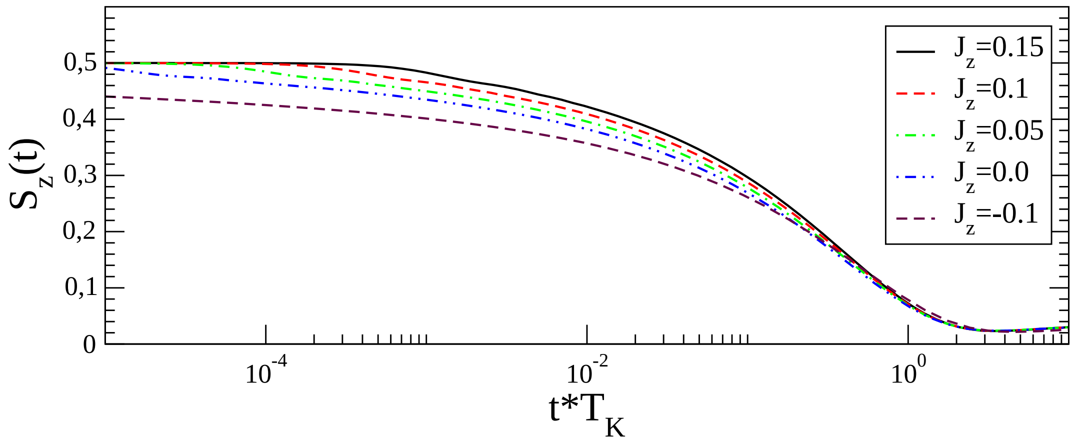

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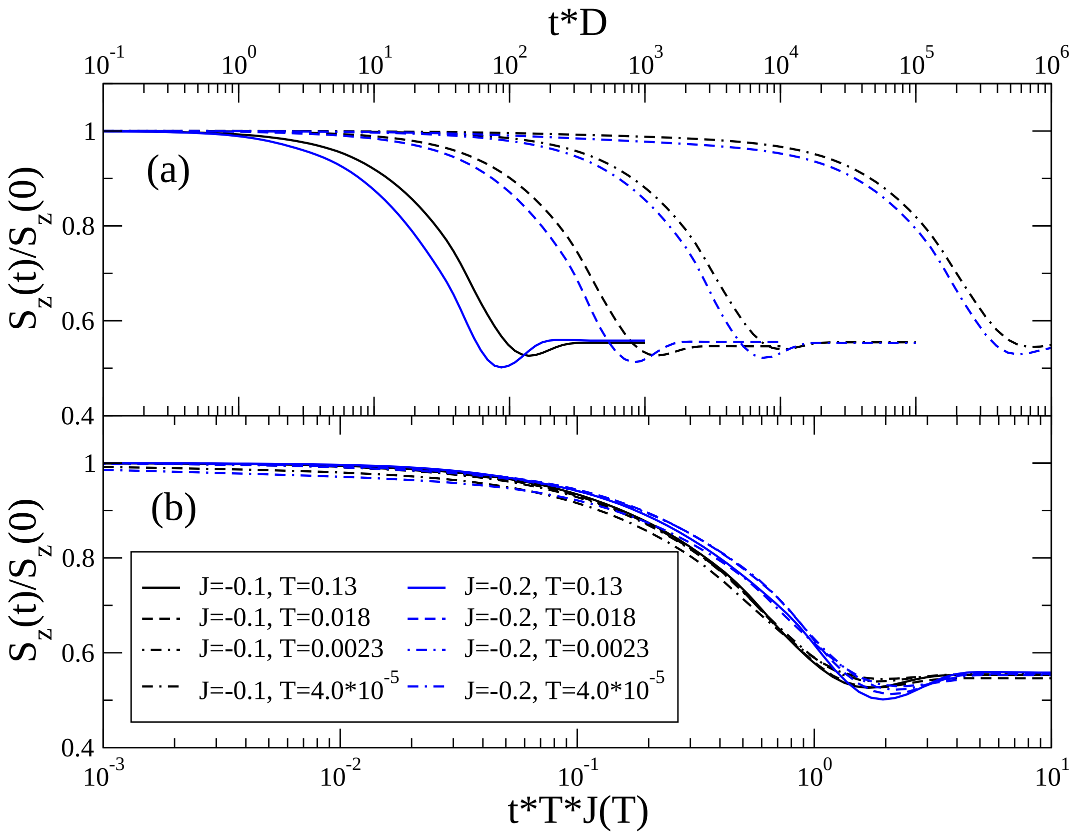
$$G(x) = \sum_{l=1}^{\infty} \frac{(-1)^{l+1}}{(2l)!2l(2l-1)} x^{2l}$$

- long time:
  $t_{long} \propto 1/T_K$

Anisotropic Kondo Model

ferromagnetic regime, spin relaxation: $H_z = 0.01 \to 0$



external magnetic field: z-axis