Relaxation Dynamics in Quantum Dot Systems Coupled to Fermionic Baths

(Project B7)

UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Lukas Litzba[1,2], Eric Kleinherbers[1,2], Friedemann Queisser[3], Gernot Schaller[3], Nikodem Szpak[1,2], Jürgen König[1,2] and Ralf Schützhold[3,4]

[1]Fakultät für Physik, Universität Duisburg Essen
[2]CENIDE, Universität Duisburg-Essen, Duisburg
[3]Helmholtz-Zentrum Dresden-Rossendorf
[4]Institut für Theoretische Physik, Technische Universität Dresden

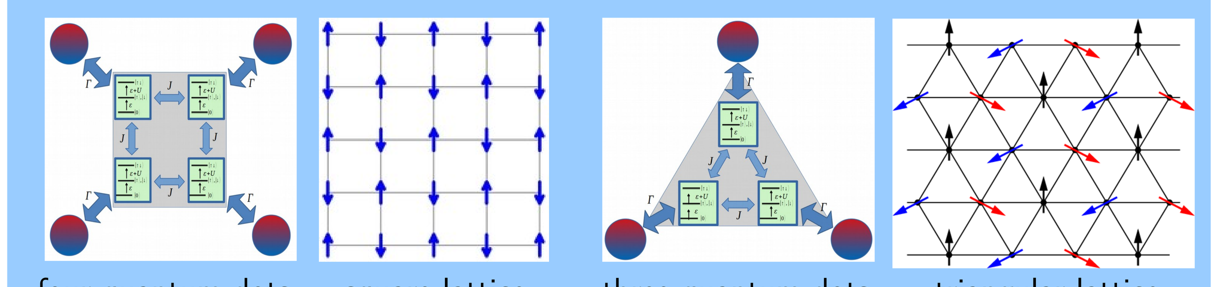
Abstract

We study the influence of the environment represented by the Markovian fermionic baths on strongly interacting quantum systems consisting of up to four quantum dots. Starting with an *ab initio* approach, we derive the Lindblad master equation describing the effective dissipation in the quantum systems within several approaches: local and global, secular and coherent [1,2]. At low temperatures, depending on the coupling parameters, the system of four dots attains or loses the antiferromagnetic order [2]. In three quantum dots, the system becomes spin-frustrated and settles down to a stable persistent spin current. Improving the theory further, we find an effective description that replaces the static bath temperature with a dynamic one, T(t), which reflects the sudden switch-on of the system-environment interaction. The effective time-dependent temperature T(t) gets high at early times and falls asymptotically to the true environment temperature T at late times. We demonstrate possible physical effects and address their measurability.

CRC 1242

Motivation

- Relaxation in open quantum systems generally complicated
- Dynamics depends strongly on interaction with environment
- Various relaxation mechanisms and time-scales



Model

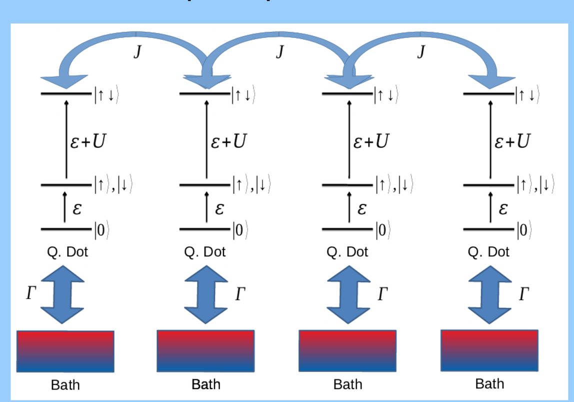
- Fermi-Hubbard model with onsite Coulomb interaction

$$H_s = -J \sum_{\langle m,m'\rangle,\sigma} c^\dagger_{m,\sigma} c_{m',\sigma} + U \sum_m n_{m,\downarrow} n_{m,\uparrow} + \varepsilon \sum_{m,\sigma} n_{m,\sigma}$$

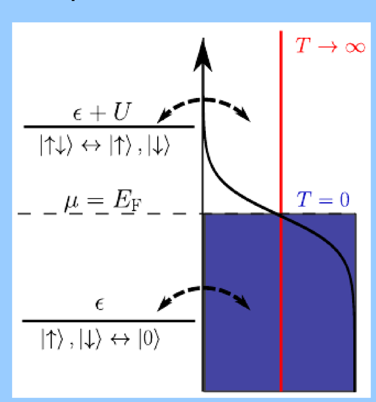
$$H_b = \sum_{k,\sigma} \varepsilon_{k,\sigma} a^\dagger_{m,k,\sigma} a_{m,k,\sigma} \qquad H_c = \sum_{m,k,\sigma} t_{k,\sigma} c^\dagger_{m,\sigma} a_{m,k,\sigma} + \text{h.c.}$$

Tunneling between sites (J) + On-site interaction (U) + On-site energy (ε)

Coupled quantum dots



Coupled to fermionic baths



Reduction to Lindblad Master equation

Tracing out bath degrees of freedom (lowest order in Γ, Markov I)
→ Redfield master equation for density matrix

$$\partial_t \hat\rho = -i[\hat H, \rho] + \sum_{n,\sigma,\pm} \gamma^\pm_{n,\sigma} \hat{\mathcal{L}}^\pm_{n,\sigma} \hat\rho$$

$\gamma^\pm_{n,l}$ couplings between system and baths, $\mathcal{L}^\pm_{n,\sigma}$ dissipators (not positive definite)

secular or coherent approximation → Lindblad operators: positive $\mathcal{L}^\pm_{n,\sigma}$

$$\hat{\mathcal{L}}^\pm_{n,l}\hat\rho = \hat L^\pm_{n,l}\hat\rho(\hat L^\pm_{n,l})^\dagger - \frac{1}{2}\{(\hat L^\pm_{n,l})^\dagger \hat L^\pm_{n,l}, \hat\rho\}$$

Global vs local approximation [1]

Global Lindblad operators (w.r.t. system eigenstates)

- secular

$$L^\pm_{m,s}(\Delta E) = \sum_{i,j} \delta_{\Delta E, E_i - E_j} \sqrt{f_\pm(E_i - E_j)}\, |\chi_i\rangle\langle\chi_i| c^\pm_{m,s} |\chi_j\rangle\langle\chi_j|$$

- coherent

$$L^\pm_{m,s} = \sum_{i,j} \sqrt{f_\pm(E_i - E_j)}\, |\chi_i\rangle\langle\chi_i| c^\pm_{m,s} |\chi_j\rangle\langle\chi_j|$$

Local Lindblad operators (w.r.t. local sites)

- secular

$$L^\alpha_{\sigma,1} = \sqrt{f_\alpha(\varepsilon)} c^\alpha_\sigma (1 - n_{\bar\sigma}),$$
$$L^\alpha_{\sigma,2} = \sqrt{f_\alpha(\varepsilon + U)} c^\alpha_\sigma n_{\bar\sigma}.$$

- coherent

$$L^\alpha_\sigma = L^\alpha_{\sigma,1} + L^\alpha_{\sigma,2} = \sqrt{f_\alpha(\varepsilon)} c^\alpha_\sigma (1 - n_{\bar\sigma}) + \sqrt{f_\alpha(\varepsilon+U)} c^\alpha_\sigma n_{\bar\sigma}$$

- for hot baths (T=∞)

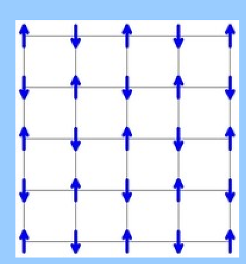
$$L^+_{m,\sigma} = c^\dagger_{m,\sigma}, \quad L^-_{m,\sigma} = c_{m,\sigma}$$

- for cold baths (T=0)

$$L^+_{m,\sigma} = c^\dagger_{m,\sigma}(1 - n_{m,\bar\sigma}), \quad L^-_{m,\sigma} = c_{m,\sigma} n_{m,\bar\sigma}$$

Square lattice – Tetramer

Fermi-Hubbard model on square lattice



For $U \gg J, \Gamma$ and $\varepsilon = -U/2 < 0$
→ low energy sector: half filling
→ Schrieffer-Wolff transf. → Heisenberg model:

$$H_{\text{eff}} = E_0 + \frac{4J^2}{U} \sum_{\langle m,n\rangle} \vec S_m \cdot \vec S_n$$

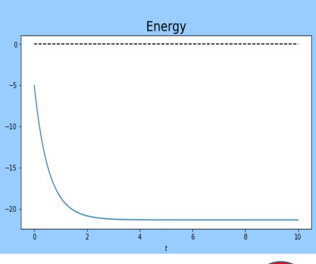
AF order preferred
coupling to environment: relaxation to AF?
→ study for N = 4

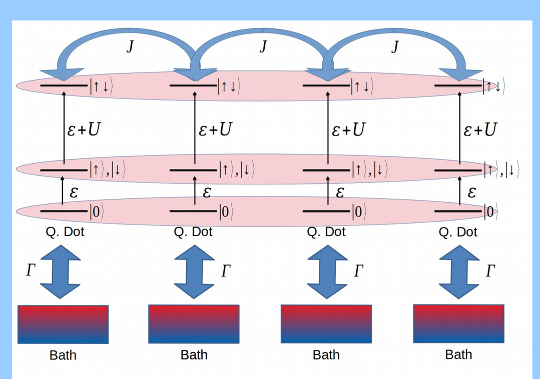
→ spin hopping + spin order parameter

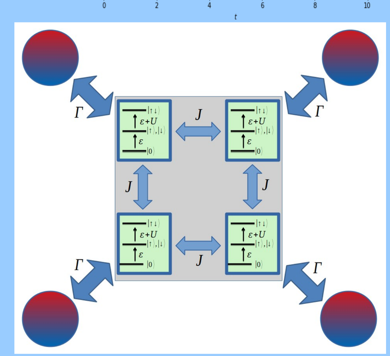
Tetramer (N=4 Quantum Dots)

- Global Lindblads (J≫Γ) → relaxation to ground state

$$|\Psi_{af}\rangle = \frac{1}{\sqrt{12}}[2|\uparrow\downarrow\uparrow\downarrow\rangle + 2|\downarrow\uparrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle]$$





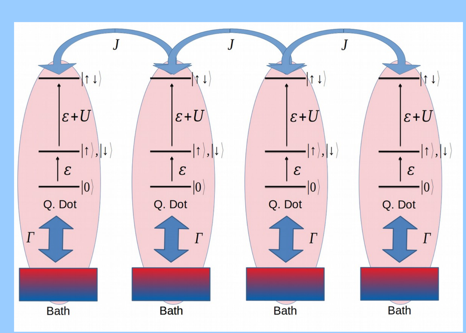


- Local Lindblads (Γ≫J): Relaxation to low energy sector
  → final state depends on the couplings
- Decay via Mott-Neel anti-ferromagnetic order (S=0)

$$|\Psi_{af}\rangle = \frac{1}{\sqrt{12}}[2|\uparrow\downarrow\uparrow\downarrow\rangle + 2|\downarrow\uparrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle]$$

- and via Ising anti-ferromagnetic order (S=1)

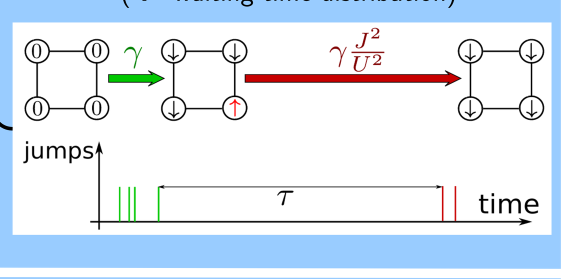
$$|\Psi_{saf}\rangle = \frac{|\uparrow\downarrow\uparrow\downarrow\rangle - |\downarrow\uparrow\downarrow\uparrow\rangle}{\sqrt2}$$



→ Final states of evolution: ferromagnetic (S=2)

$$|\Psi_{-2}\rangle = |\downarrow\downarrow\downarrow\downarrow\rangle$$
$$|\Psi_{-1}\rangle = \frac12[|\uparrow\downarrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\downarrow\uparrow\rangle]$$
$$|\Psi_0\rangle = \frac{1}{\sqrt6}[|\uparrow\uparrow\downarrow\downarrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle]$$
$$|\Psi_{+1}\rangle = \frac12[|\downarrow\uparrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\uparrow\downarrow\rangle]$$
$$|\Psi_{+2}\rangle = |\uparrow\uparrow\uparrow\uparrow\rangle$$

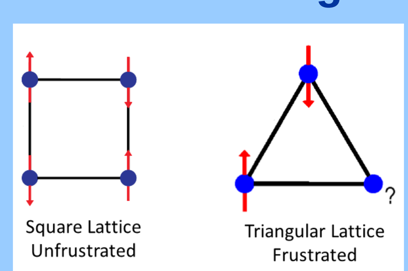
Relaxation via classically forbidden processes
(→ waiting time distribution)

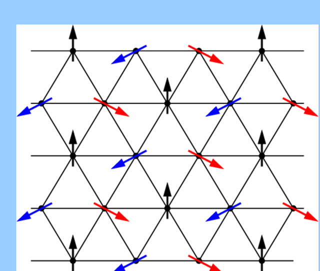


Triangular lattice – Trimer

Fermi-Hubbard model on triangular lattice

→ AF order preferred but impossible
→ spin frustration
→ spin waves

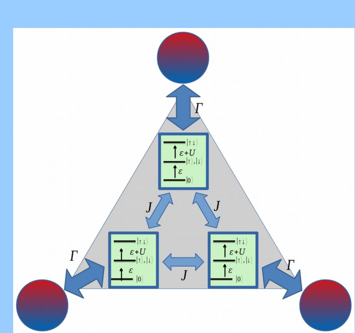




Trimer (N=3 Quantum Dots)

Steady states at low energy:

1. $|\uparrow,\uparrow,\uparrow\rangle$ $(S_z = \frac32)$
2. 3 states with $\uparrow,\uparrow$ and $\downarrow$ $(S_z = \frac12)$
3. 3 states with $\downarrow,\downarrow$ and $\uparrow$ $(S_z = -\frac12)$
4. $|\downarrow,\downarrow,\downarrow\rangle$ $(S_z = -\frac32)$



Spin waves

$$|S_0\rangle = \frac{1}{\sqrt3}\left[|\uparrow,\downarrow,\downarrow\rangle + |\downarrow,\uparrow,\downarrow\rangle + |\downarrow,\downarrow,\uparrow\rangle\right]$$
$$|S_+\rangle = \frac{1}{\sqrt3}\left[|\uparrow,\downarrow,\downarrow\rangle + e^{ik_0}|\downarrow,\uparrow,\downarrow\rangle + e^{-ik_0}|\downarrow,\downarrow,\uparrow\rangle\right]$$
$$|S_-\rangle = \frac{1}{\sqrt3}\left[|\uparrow,\downarrow,\downarrow\rangle + e^{-ik_0}|\downarrow,\uparrow,\downarrow\rangle + e^{ik_0}|\downarrow,\downarrow,\uparrow\rangle\right] \qquad k_0 = 2\pi/3$$

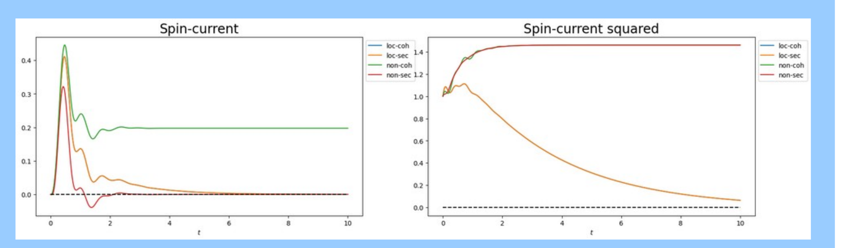
→ spin waves with non-zero spin current ~ ground states!

Relaxation to spin currents

From: $|\psi_0\rangle = |\uparrow, 0, \downarrow\rangle$

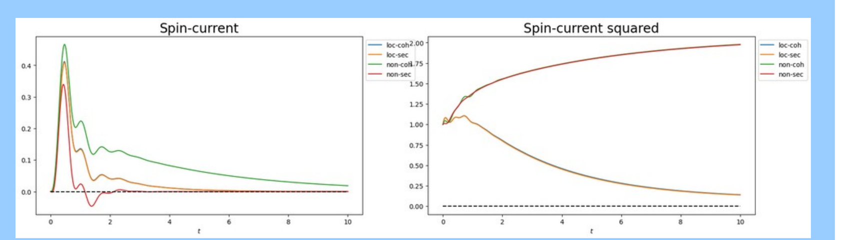
- T=0

spin current right > spin current left



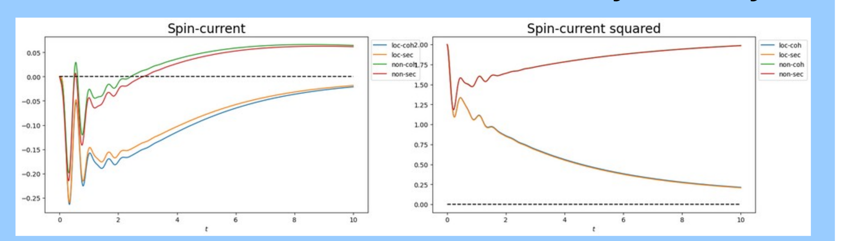
- T ≥ 0 (T ~ Γ)

spin current right = spin current left

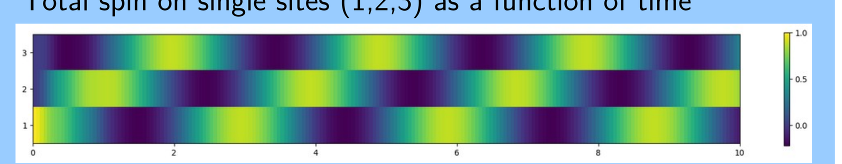


- T ≥ 0 + Magnetic flux: B > 0 → breaks the L-R symmetry

spin current right > spin current left



Total spin on single sites (1,2,3) as a function of time



Time-dependent temperature model

Static Lindblad operators obtain coefficients from the Fermi-Dirac distribution (Infinite history; Fermi-Dirac distribution)

$$\gamma_{T,\Delta E} = \frac12 \pm \int_0^\infty T\frac{\sin(\Delta E\tau)}{\sinh(\pi T\tau)}d\tau = \frac12 \pm \frac12\tanh\left(\frac{\Delta E}{2T}\right) = \frac{1}{1+e^{\mp\Delta E/T}} = f_T(\mp\Delta E)$$

Here: t = ∞ follows from infinite history ⇐ simplifying assumption (Markov II)

Exact

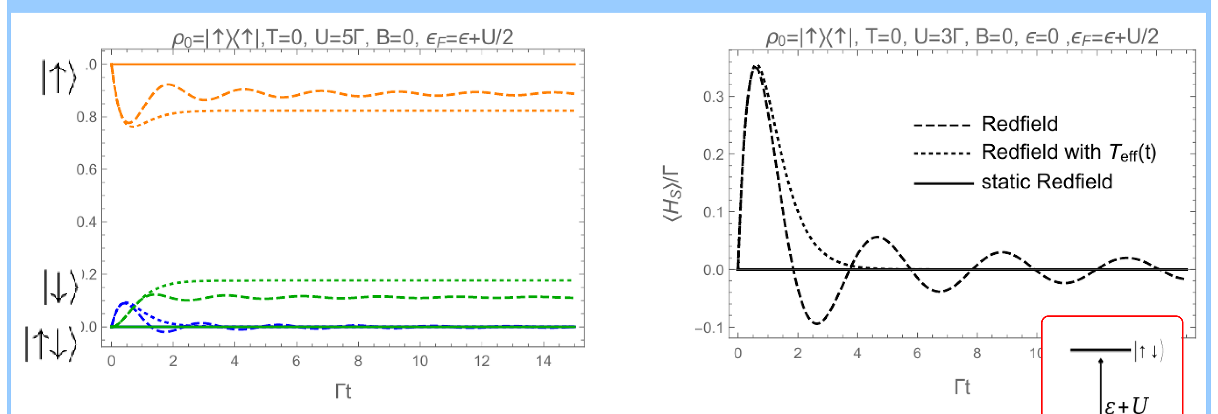
$$F_{T,\Delta E}(t) = \int_0^t T\frac{\sin(\Delta E\tau)}{\sinh(\pi T\tau)}d\tau \approx \frac12\tanh\left[\frac{\Delta E}{2T}\tanh\left(\frac{4Tt}{\pi}\right)\right]$$

→ Uniform approximation for all parameters: T, ΔE, t ! (with oscillations avergaged out)

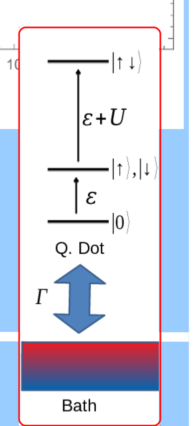
We get $\gamma_{T,\Delta E} = \frac12 \pm F_{T,\Delta E}(t) \approx f_{T(t)}(\mp\Delta E)$ with $T(t) = \frac{T}{\tanh(4Tt/\pi)}$

→ looks like thermal with time-dependent temperature T(t) !

One quantum dot coupled to cold bath



- Full Redfield: negative probabilities and negative energy
- Redfield with T(t): positive probabilities and positive energy
- Static Redfield: no dynamics



Conclusions

Differences among approximation schemes, depending on system parameters regime

- Anti-ferromagnetic order (N=2, N=4):
  - strong coupling to env. (local): AF **metastable** → ferromagnetic
  - weak coupling to env. (global): AF **stable**
- Persistent spin currents (N=3)
  - strong coupling to env. (local): spin **currents decay**
  - weak coupling to env. (global secular): only **symmetric currents**
  - weak coupling to env. (global coherent): **asymmetric currents**
- Time-dependent effective temperature T(t) (N=1)
  - static T: **no dynamics**
  - T(t): **quench dynamics**

Collaborative Research Centre 1242

Non-Equilibrium Dynamics of Condensed Matter in the Time Domain

Gefördert durch DFG Deutsche Forschungsgemeinschaft

Publications:
1. E. Kleinherbers, N. Szpak, J. König, R. Schützhold, Phys. Rev. B 101, 125131 (2020)
2. G. Schaller, F. Queisser, N. Szpak, J. König, and R. Schützhold, Phys. Rev. B 105, 115139 (2022)

E-mail: nikodem.szpak@uni-due.de