A non-equilibrium Dynamical Mean Field Theory approach based on the Lindblad equation

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Introduction

Strongly correlated systems far from equilibrium:

- Transport through quantum dots, molecules or heterostructures
- Ultracold atoms, cavity arrays
- Ultrafast laser spectroscopy

Theoretical approaches, e.g.: Quantum Monte Carlo (Eckstein 09), Functional Renormalisation Group (Graz, Jakobs 07), Numerical RG (Anders 08), Density-Matrix RG (White 04, Schollwöck, Heidrich-Meisner), CPT/VCA (Balzer 11, Knap 11), DMFT (Schmidt, Monien 02, Freericks, Turkowski, Zlati 06).

Non-equilibrium description in the framework of Keldysh Green’s functions:

- Stationary state given by eigenvector $\rho_{eq}$
- Theoretical approaches, e.g.: Quantum Monte Carlo (Eckstein 09), Functional
- Renormalisation Group (Graz, Jakobs 07), Numerical RG (Anders 08), Density-Matrix RG (White 04, Schollwöck, Heidrich-Meisner), CPT/VCA (Balzer 11, Knap 11), DMFT (Schmidt, Monien 02, Freericks, Turkowski, Zlati 06).

- Numerical solution:
  - Calculation of Green’s functions by a two-sided Lanczos iteration with biorthogonalization of left- and right-sided vectors.
  - Exact diagonalisation of an effective Lindblad quantum Master equation with absorbing boundaries allows for direct calculation of steady states.
  - Super-Fock space much larger but also increased number of fit parameters, quick convergence with cluster size $N$.
  - Current-voltage characteristics agree well with Time Evolving Block Decimation (TEBD) and non-equ. Variational Cluster Approach (nVCA) [6, 7].

Method

**Effective impurity problem** [2]: Impurity coupled to two non-interacting chains with additional Markovian baths.

- Infinite, dissipative system, thus allowing for long time evolutions and treatment of steady states.

Lindblad quantum master equation for the (reduced) density matrix [3]:

$$\frac{d}{dt} \rho = (\mathcal{L}_B + \mathcal{L}_I) \rho,$$

with

$$\mathcal{L}_B \rho = -i[H, \rho] - \sum_{n,m} E_{n,m} \rho_{n,m} \rho_{\bar{n},\bar{m}} + \Gamma \rho_{\bar{n},\bar{m}},$$

$$\mathcal{L}_I \rho = 2 \sum_{n,m} \left[ \Gamma^{\uparrow}_{n,m} \left( \rho_{n,m} \rho_{\bar{n},\bar{m}} - \frac{1}{2} \rho_{n,m} \rho_{\bar{n},\bar{m}} \right) + \Gamma^{\downarrow}_{n,m} \left( \rho_{n,m} \rho_{\bar{n},\bar{m}} - \frac{1}{2} \rho_{n,m} \rho_{\bar{n},\bar{m}} \right) \right].$$

Bath parameters $E_{n,m}$ and $\Gamma^{\uparrow}_{n,m}$ and $\Gamma^{\downarrow}_{n,m}$ adjusted to the physical system and determined by minimizing the cost function

$$\sum_{i,t} \left| \langle \Delta^i (\omega) \rangle - \Delta^i (\omega) \rangle \right| d\omega.$$ 

Super-Fock representation [4]: Introducing super-Fock states $\langle \{n\} \rangle \otimes \{\{\bar{n}\}\}$, with twice as many fermions, enables one to rewrite the Lindblad equation in a non-hermitian Hamiltonian form:

$$\frac{d}{dt} \rho = [\mathcal{H}, \rho],$$

with

$$\mathcal{H} = \sum_{n,m} E_{n,m} \rho_{n,m} \rho_{\bar{n},\bar{m}} + \Gamma \rho_{\bar{n},\bar{m}},$$

$$\mathcal{L}_I \rho = 2 \sum_{n,m} \left[ \Gamma^{\uparrow}_{n,m} \left( \rho_{n,m} \rho_{\bar{n},\bar{m}} - \frac{1}{2} \rho_{n,m} \rho_{\bar{n},\bar{m}} \right) + \Gamma^{\downarrow}_{n,m} \left( \rho_{n,m} \rho_{\bar{n},\bar{m}} - \frac{1}{2} \rho_{n,m} \rho_{\bar{n},\bar{m}} \right) \right].$$

Numerical solution:

- The steady state is determined by applying a (hermitian) Lanczos scheme to $\mathcal{L}_I \rho$.
- Calculation of Green’s functions by a two-sided Lanczos iteration with biorthogonalization of left- and right-sided vectors.

Discussion

References


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