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

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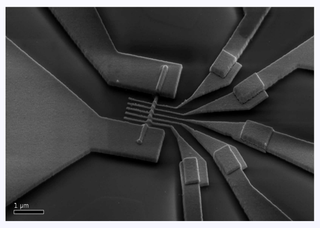
Introduction

Strongly correlated systems far from equilibrium:

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



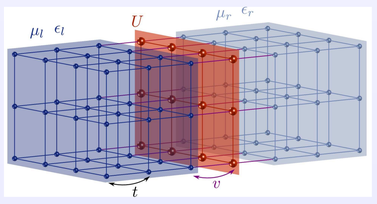
Theoretical approaches, e.g.: Quantum Monte Carlo (Eckstein 09), Functional Renormalisation Group (Gezzi, Jakobs 07), Numerical RG (Anders 08), Density-Matrix RG (White 04, Schollwöck, Heidrich-Meisner), CPT/VCA (Balzer 11, Knap 11), DMFT (Schmidt, Monien 02, Freericks, Turkowski, Zlati 06).

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

$$\underline{G}(\mathbf{k},\omega) = \begin{pmatrix} G^{\mathrm{R}}(\mathbf{k},\omega) & G^{\mathrm{K}}(\mathbf{k},\omega) \\ 0 & G^{\mathrm{A}}(\mathbf{k},\omega) \end{pmatrix} \tag{1}$$

Transport through an interacting layer:

- (non-interacting) Green's functions of the central region: $\underline{g}_0(\mathbf{k}_\parallel,\omega)$
- GFs of decoupled leads: $\underline{g}_\alpha(\mathbf{k}_\parallel,\omega)$
- Full GF of the central region:



$$\underline{G}^{-1}(\mathbf{k}_\parallel,\omega) = \underline{g}_0^{-1}(\mathbf{k}_\parallel,\omega) - \sum_{\alpha=\mathrm{l,r}} |v|^2 \underline{g}_\alpha(\mathbf{k}_\parallel,\omega) - \underline{\Sigma}(\mathbf{k}_\parallel,\omega) \tag{2}$$

Dynamical Mean Field Theory (DMFT) [1]: Approximate self energy $\underline{\Sigma}(\mathbf{k}_\parallel,\omega)$ by a local $\underline{\Sigma}_{LOC}(\omega)$, obtained from an effective non-equilibrium impurity problem:

$$\underline{G}^{-1}_{IMP}(\omega) = \underline{g}_0^{-1}(\omega) - \underline{\Delta}(\omega) - \underline{\Sigma}_{LOC}(\omega) \tag{3}$$

Bath hybridization function $\underline{\Delta}(\omega)$ determined by the self-consistency condition

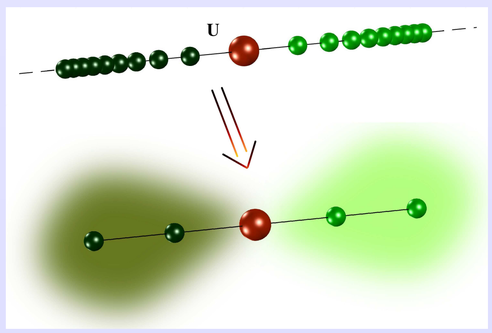
$$\underline{G}_{LOC}(\omega) = \underline{G}_{IMP}(\omega)\,, \tag{4}$$

with $\underline{G}_{LOC}(\omega) = \frac{1}{(2\pi)^2}\int \underline{G}(\mathbf{k}_\parallel,\omega) d\mathbf{k}_\parallel$, the local Green's function of the layer.

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]:

$$\frac{d}{d\tau}\rho = (\mathcal{L}_H + \mathcal{L}_b)\,\rho\,, \quad \text{with} \tag{5}$$

$$\mathcal{L}_H\rho = -i[H,\rho]\,, \quad H = \sum_{n,m,\sigma} E_{n,m} c^\dagger_{n\sigma} c_{m\sigma} + U n_{0\uparrow} n_{0\downarrow}\,, \tag{6}$$

$$\mathcal{L}_b\rho = 2\sum_{n,m,\sigma}\left[\Gamma^{(1)}_{n,m}\left(c_{n\sigma}\rho c^\dagger_{m\sigma} - \frac{1}{2}\{c^\dagger_{m\sigma}c_{n\sigma},\rho\}\right) + \Gamma^{(2)}_{n,m}\left(c^\dagger_{n\sigma}\rho c_{m\sigma} - \frac{1}{2}\{c_{m\sigma}c^\dagger_{n\sigma},\rho\}\right)\right] \tag{7}$$

Bath parameters $E_{n,m}$, $\Gamma^{(1)}_{n,m}$ and $\Gamma^{(2)}_{n,m}$ adjusted to the physical system and determined by minimizing the cost function $\sum_{x=\mathrm{R,K}}\int||\underline{\Delta}^x(\omega) - \underline{\Delta}^x_{eff}(\omega)||d\omega$.

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

$$\frac{d}{d\tau}|\rho\rangle = L|\rho\rangle \tag{8}$$

① Stationary state given by eigenvector $|\rho_{\mathrm{s.s.}}\rangle$ of L with eigenvalue zero.

② Green's functions calculated via the quantum regression theorem [3]:

$$\frac{d}{d\tau}c(\tau-\tau')\rho(\tau') = \mathcal{L}\left(c(\tau-\tau')\rho(\tau')\right) \tag{9}$$

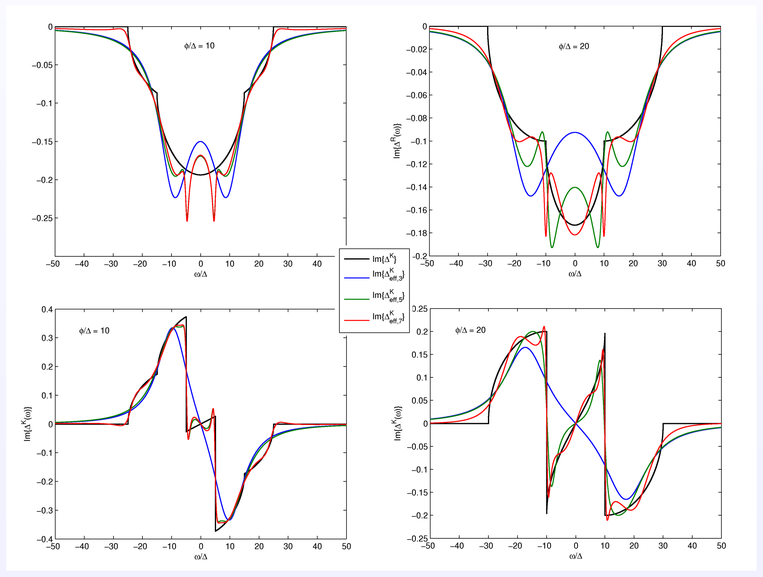
Numerical solution :

❶ The steady state is determined by applying a (hermitian) Lanczos scheme to $L^\dagger L$.

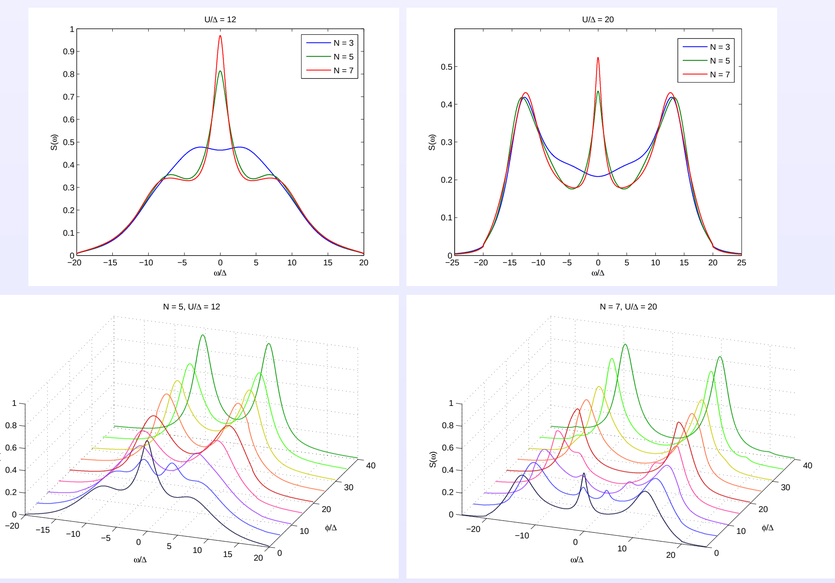
❷ Calculation of Green's functions by a two-sided Lanczos iteration with biorthogonalization of left- and right-sided vectors.

Benchmark: Single Impurity Anderson Model [5]

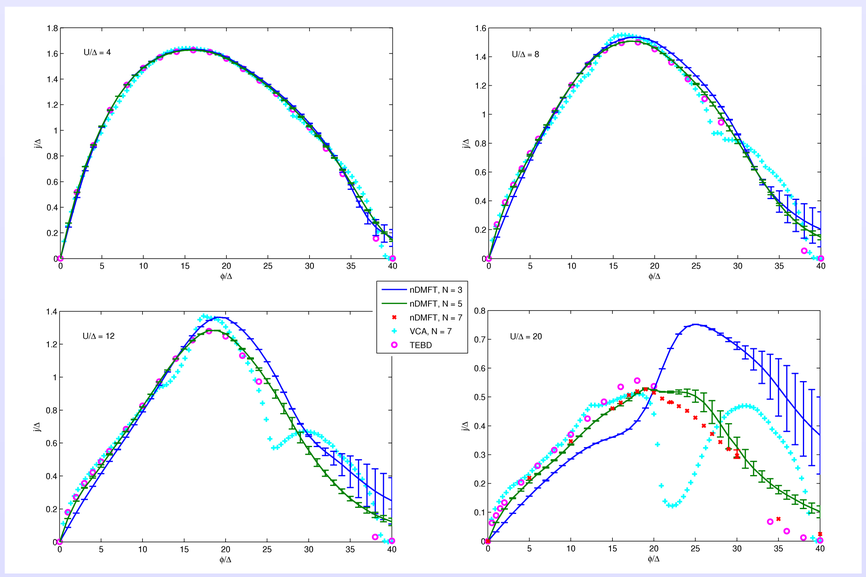
❒ **Fit of hybridization function**



❒ **Single particle spectral function: Equilibrium case and bias-dependent**



❒ **Current-voltage characteristics**



Discussion

➤ 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-eq. Variational Cluster Approach (nVCA) [6, 7].

References

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