Auxiliary Master Equation for Nonequilibrium Dual Fermion Approach

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Abstract

We introduce an auxiliary quantum master equation (QME) dual fermion (Aux-DF) method and argue that it presents a convenient way to describe steady states of correlated impurity models. The scheme yields an expansion around a reference that is much closer to the true nonequilibrium state than that in the original dual fermion (DF) formulation. In steady-state situations, the scheme is numerically inexpensive and avoids time propagation. The Anderson impurity model (AIM) is used to test the approach against numerically exact benchmarks: time-dependent density matrix renormalization group (td-DMRG) and continuous time quantum Monte Carlo (CT-QMC).

Original DF Formulation

Originally, the DF method was formulated for equilibrium lattice models as a way to account for nonlocal correlations beyond DMFT [1]. A nonequilibrium version of the method (DF-inspired superperturbation theory) was later proposed in Ref. [2] as a way to solve impurity transport problems.

At the heart of the approach is **finite reference system**, which includes the molecule and a finite number of states representing leads. The reference problem can be solved exactly. DF is an expansion accounts for the difference between the true system-lead hybridization and its approximation within the reference system.

$$S[d^*,d] = \sum_{1,2} d_1^* \left[G_0^{-1} - \Sigma^B\right]_{12} d_2 + S^{int}[d^*,d]$$
$$= \tilde{S}[d^*,d] + \sum_{1,2} d_1^* \left[\tilde{\Sigma}^B_{12} - \Sigma^B_{12}\right] d_2$$

Hubbard-Startonovich transformation $\rightarrow$ **dual fermion (DF)**

$$S^{DF}[f^*,f] = \sum_{1,2} f_1^* \left[(G_0^{DF})^{-1} - \Sigma^{DF}\right]_{12} f_2$$
$$\left(G_0^{DF}\right)^{-1}_{12} = -g^{-1}_{12} - \sum_{3,4} g^{-1}_{13} \left[\tilde{\Sigma}^B - \Sigma^B\right]^{-1}_{34} g^{-1}_{42},$$
$$\Sigma^{DF}_{12} = \sum_{3,4} \Gamma_{13;24} \left[G_0^{DF}\right]_{43}.$$

g_{12} and $\Gamma_{13;24}$ are the single-particle GF and the two-particle vertex of the reference system. The single-particle GF of the molecule is obtained from

$$G = \left(\delta\Sigma^B\right)^{-1} + \left[g\,\delta\Sigma^B\right]^{-1} G^{DF} \left[\delta\Sigma^B\, g\right]^{-1}; \qquad \delta\Sigma^B \equiv \tilde{\Sigma}^B - \Sigma^B$$

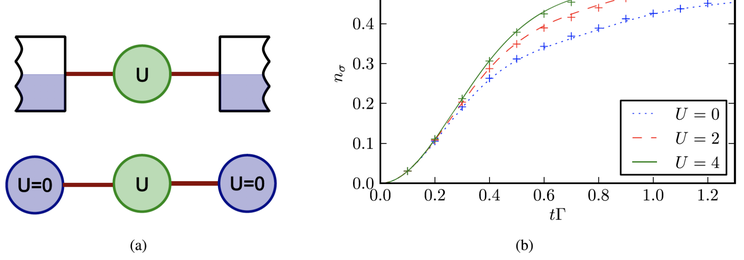

Figure 1: (a) original and reference systems; (b) time evolution of the level occupation after coupling to baths (no bias). From Ref. [2].

Deficiencies of the Original DF

Where the steady-state is of interest, the original DF is problematic:

- Few sites representing bath yield hybridization function significantly different from the true one
- Finite reference system $\rightarrow$ periodic solution, so that reaching the steady-state requires long time propagation

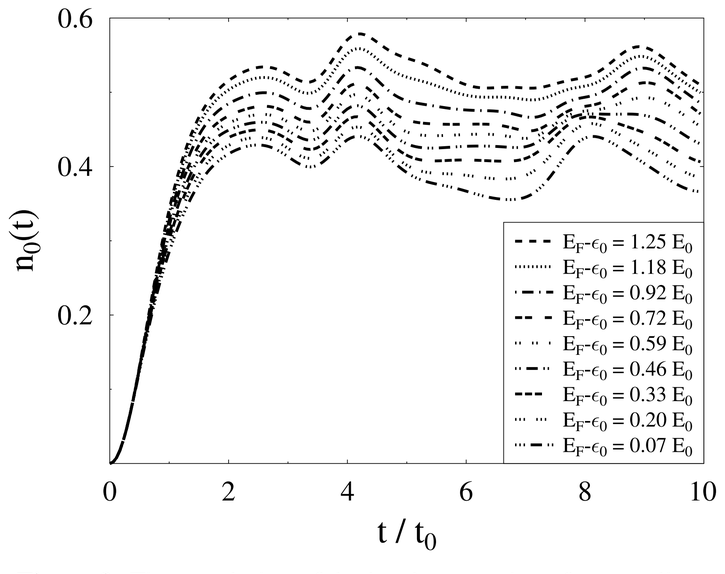

Figure 2: Time evolution of the level occupation after coupling to baths (biased junction). From Ref. [3]

Aux-DF Method

In Ref. [3] we proposed to introduce **infinite reference system**

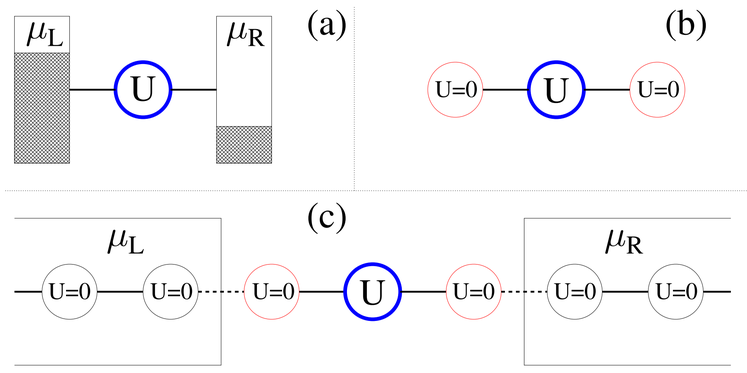

Figure 3: (a) AIM and corresponding reference systems in (b) DF and (c) Aux-DF methods. From Ref. [3].

and to solve it using **auxiliary QME**

$$\frac{d\rho^S(t)}{dt} = -i\mathcal{L}\rho^S(t)$$

GF and vertex for the reference system are simulated using the quantum regression relation

$$\left\langle T_c\, \hat{A}(\tau_1)\, \hat{B}(\tau_2) \ldots \hat{Z}(\tau_n)\right\rangle =$$
$$\mathrm{Tr}\left[\mathcal{O}_n \mathcal{U}(t_n, t_{n-1}) \ldots \mathcal{O}_2 \mathcal{U}(t_2,t_1)\, \mathcal{O}_1 \mathcal{U}(t_1,0)\, \rho^S(0)\right]$$

Here $\rho^S(0)$ is the steady-state density matrix of the extended system, $\mathcal{U}(t_i,t_{i-1})$ is the Liouville space evolution operator and times t_i are ordered so that $t_n > t_{n-1} > \ldots > t_2 > t_1 > 0$. $\mathcal{O}_i$ is the Liouville space super-operator corresponding to one of operators $\hat{A} \ldots \hat{Z}$ whose time is i-th in the ordering. It acts from the left (right) for the operator on the forward (backward) branch of the contour. The steady-state density matrix is found as a right eigenvector $|R_0 \gg$ corresponding to the Liouvillian eigenvalue $\lambda_0 = 0$.

Using spectral decomposition of the Liouvillian, the evolution operator can be presented in its eigenbasis as

$$\mathcal{U}(t_i,t_{i-1}) = \sum_\gamma |R_\gamma \gg\, e^{-i\lambda_\gamma (t_i - t_{i-1})}\, \ll L_\gamma|.$$

Once single- (g) and two-particle ($g^{(2)}$) GFs of the reference system are known, the vertex required in DF formulation is given by

$$\Gamma_{13;24} = \sum_{\substack{1',2'\\3',4'}} g^{-1}_{11'}\, g^{-1}_{33'} \left[g^{(2)}_{1'3';2'4'} - g_{1'2'}\, g_{3'4'} + g_{1'4'}\, g_{3'2'}\right] g^{-1}_{2'2}\, g^{-1}_{4'4}.$$

Numerical Benchmarks for the Aux-DF

We apply the Aux-DF method to the AIM

$$\hat{H} = \hat{H}_M + \sum_{K=L,R} \left(\hat{H}_K + \hat{V}_{MK}\right)$$

where

$$\hat{H}_M = \sum_{\sigma=\uparrow,\downarrow} \epsilon_0\, \hat{d}^\dagger_\sigma \hat{d}_\sigma + U \hat{n}_\uparrow \hat{n}_\downarrow$$
$$\hat{H}_K = \sum_{k\in K} \sum_{\sigma=\uparrow,\downarrow} \epsilon_k\, \hat{c}^\dagger_{k\sigma} \hat{c}_{k\sigma}$$
$$\hat{V}_{MK} = \sum_{k\in K} \sum_{\sigma=\uparrow,\downarrow} \left(V_k \hat{d}^\dagger_\sigma \hat{c}_{k\sigma} + H.c.\right)$$

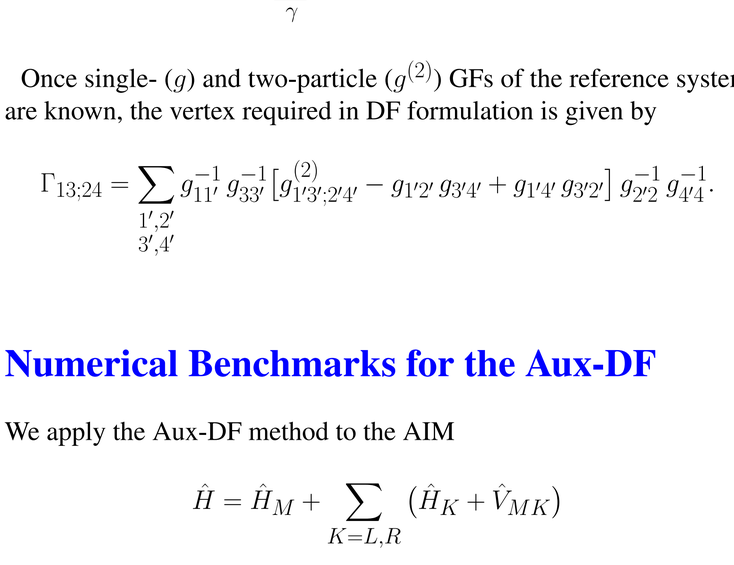

Figure 4: Current voltage characteristics simulated within QME (dotted line), zero (dashed line) and first (solid line) order Aux-DF approaches. Circles and squares represent respectively tdDMRG and CT-QMC results. From Ref. [3].

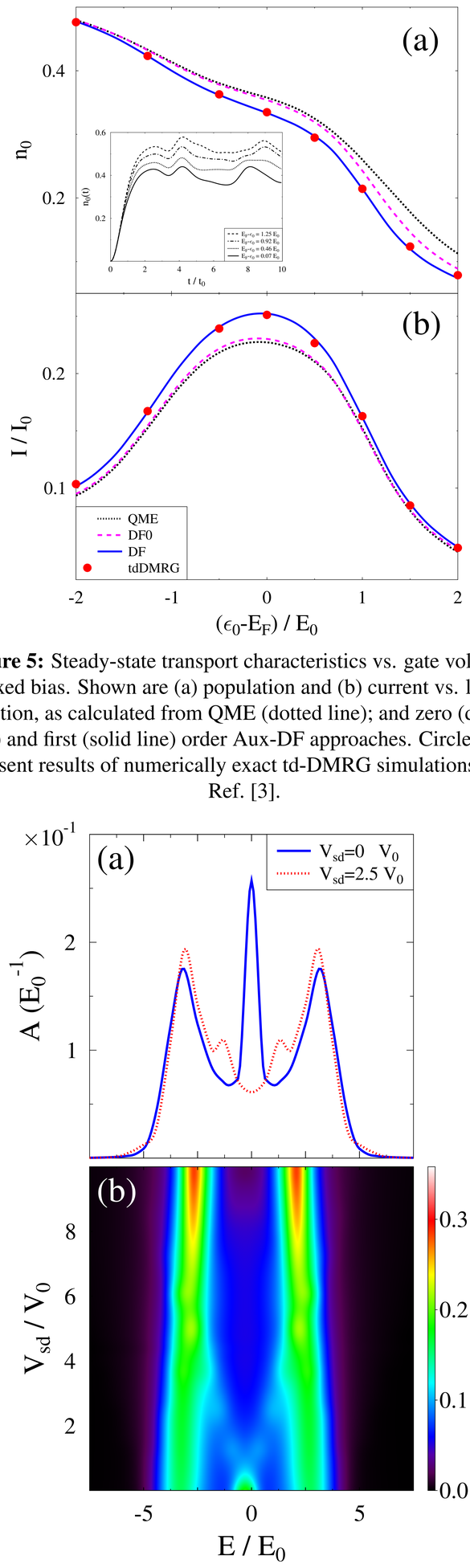

Figure 5: Steady-state transport characteristics vs. gate voltage at fixed bias. Shown are (a) population and (b) current vs. level position, as calculated from QME (dotted line); and zero (dashed line) and first (solid line) order Aux-DF approaches. Circles (red) represent results of numerically exact td-DMRG simulations. From Ref. [3].

Figure 6:. Spectral function of Anderson impurity model. Shown are results of Aux-DF simulations for (a) The spectral function of the unbiased (solid line) and biased (dotted line) junction; and (b) The spectral function vs. energy and applied bias. From Ref. [3].

Conclusions

We introduce Aux-DF method for simulation of strongly correlated open nonequilibrium systems. Finite reference reference system of the original DF formulation is substituted with an infinite open system which is solved using auxiliary QME. This allows more realistic treatment of dissipation and yields information on nonequilibirum state of the system. Aux-DF allows to avoid long time propagations of the original DF and is advantageous in treating steady states. AIM is used as a test model and compared with numerically exact td-DMRG and CT-QMC results. Aux-DF is shown to be quite accurate and relatively inexpensive numerically.

References

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