Nonequilibrium atomic limit
Projection operators NEGF-EOM approach to quantum transport
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QUANTUM DOT: COULOMB BLOCKADE REGIME.
As our first example, we investigate a single quantum dot (QD) with a strong Coulomb interaction parameter $U$ and weak coupling to the contacts $\Gamma$.

Under these conditions the QD is close to the nonequilibrium atomic limit and the state-resolved system excitations are the right choice for our initial vector of operators.

$$\hat{A}_I = \begin{pmatrix} (1-\hbar \omega_0) \hat{n}_0, (1-\hbar \omega_0) \hat{n}_0, 2\hbar \omega_0 \hat{a}_0, 2\hbar \omega_0 \hat{a}_0 \end{pmatrix}^T$$

This Figure shows the density of states, in equilibrium (blue) and under symmetrically-applied bias (red).

Parameters for this calculation are (in units of $\Gamma$): $T=0.005$, $E_{ac}=0$, $\Gamma_{ac}=0.5$, $E_\omega=0$, splitting factor equal to $\frac{1}{2}$ and an energy grid spanning region from $-3$ to $3$.

QUANTUM DOT: KONDO REGIME.
Next, we investigate a single quantum dot (QD) with an infinitely strong Coulomb interaction and weak coupling to the contacts, then double occupancy is forbidden and the Kondo effect is the result of bath-induced correlations in the system.

Assumptions for this model lead us to choose $\Gamma_{ac}$ as the right choice for our initial vector of operators.

$$\hat{A}_I = \begin{pmatrix} (1-\hbar \omega_0) \hat{n}_0, (1-\hbar \omega_0) \hat{n}_0, 2\hbar \omega_0 \hat{a}_0, 2\hbar \omega_0 \hat{a}_0 \end{pmatrix}^T$$

This Figure shows the density of states, in equilibrium (blue) and under symmetrically-applied bias (red).

Parameters for this calculation are (in units of $\Gamma$): $T=0.001$, $E_{ac}=0.4$, $\Gamma_{ac}=-0.6$, $\Gamma_{ac}=0.01$, $E_\omega=0$. Bias is applied symmetrically with splitting factor equal to $\frac{1}{2}$ and an energy grid spanning form $-3$ to $3$.

THEORY AND METHODOLOGY
The EOM technique provides a way to study correlation functions of any set of operators

$$G_{ab}(\tau,\tau') = -i \left\langle T_a \hat{b}_a^\dagger(\tau) \hat{b}_b(\tau') \right\rangle$$

yielding (in general) an infinite chain of equations of motion. The main drawback of the method is the necessity to make uncontrolled approximations in order to truncate the chain of equations.

Uncontrolled decoupling of correlation functions may result in complications related to loss of proper commutation relations between the decoupled operators. Here we present a methodology that solves these problems.

Heisenberg EOMs introduce an infinite sequence of operators $\hat{a}_n(\tau)$

$$\frac{\partial}{\partial \tau}' \hat{a}_n(\tau) = c_n(\tau) \hat{a}_n(\tau) + \nu_{a,n+1} \hat{a}_{n+1}(\tau) + \nu_{b,n+1} \hat{b}_{n+1}(\tau)$$

Utilizing the scalar product

$$P_{ab} = \left\langle \hat{a}_n^\dagger \hat{b}_n \right\rangle$$

we orthogonalize vectors in generation $n$ relative to all previous generations

$$\hat{a}_n \Rightarrow \hat{a}_n - \sum_{m=n}^{\infty} P_{a,m}^n \hat{a}_m^\dagger \hat{a}_n^\dagger$$

Introducing irreducible Green functions

$$G^{(a)}_{n}(\tau,\tau') = \int d\tau_1 d\tau_2 G^{(a)}_{n}(\tau,\tau_1) G^{(a)}_{n}(\tau_1,\tau_2) G^{(a)}_{n}(\tau_2,\tau')$$

performing a local gauge transformation.

$$G^{(a)}_{n}(\tau,\tau') = P_{a,n}^\dagger(\tau) \left( c_n(\tau) \delta(\tau,\tau') + \int_\varepsilon d\varepsilon G^{(a)}_{n}(\tau,\varepsilon) \right) P_{a,n}^\dagger(\tau')$$

We arrive at a set of EOMs of the canonical (Dyson) type for arbitrary operators describing the system

$$\left( \frac{\partial}{\partial \tau} - \nu_{a,b} \right) G^{(a)}_{n}(\tau,\tau') = \delta(\tau,\tau_0) \hat{a}_n + \int_\varepsilon d\varepsilon G^{(a)}_{n}(\tau,\varepsilon) G^{(a)}_{n}(\varepsilon,\tau')$$

This set of equations allows for a controlled decoupling of the EOM chain and resolves symmetry violations present in the standard NEGF-EOM approaches.

TWO-LEVEL SYSTEM
We study a model for a junction with only two levels within this methodology. In this case, we describe the system in terms of Hubbard operators

$$\hat{A}_I = \begin{pmatrix} \hat{q}_0 & \hat{q}_0 & \hat{q}_2 & \hat{q}_2 \end{pmatrix}^T$$

The Figure presents simulations within the standard NEGF (red) and the projection operator scheme (blue). Shown are (a) the probabilities and (b) the coherences of the many-body eigenstates of the TLS, and (c) current vs. applied bias $V_{ac}$.

Panels (b) and (c) show also results of the Redfield QME simulation (dotted and double-dotted lines, green).

QD UNDER AN ac MAGNETIC FIELD IN KONDO REGIME
The presence of an ac magnetic field with frequency $\omega$ brings additional time-dependent dynamics. In this case, treatment within the projection operator NEGF EOM method is possible with the following choice

$$\hat{A}_I = \begin{pmatrix} \hat{q}_0 & \hat{q}_0 & \hat{q}_2 & \hat{q}_2 \end{pmatrix}^T$$

Here we illustrate (a) The density of states for $\omega=0$ spin up (red), $\omega=0$ spin down (blue) and for both with $\omega=1$ (black). (b) DOS for the spin up as a function of $\omega$ and Energy $E$.

Parameters for this calculation are (in units of $\Gamma$): $E_{ac}=2.5$, $E_{down}=-1.5$, $g=0.2$ and $V_{ac}=0$. This figure illustrates avoided crossing demonstrated by the Kondo peaks of the two densities when the frequency of the ac magnetic field approached the molecular resonance.