Fast Transients in Mesoscopic Systems

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Abstract. We study fast transient dynamics of an open quantum system at the initial stage of its equilibration starting far from equilibrium from correlated initial conditions reflecting entanglement with the environment. These correlations rapidly decay and the process enters the non-equilibrium quasi-particle mode controlled by a generalized master equation. As a model system, the nanoscopic molecular bridge between two leads is considered. The coupling to the leads is assumed to be intermittent. Properties of the resulting transients are demonstrated and analyzed.

Keywords: Molecular bridge, Initial conditions, Decay of correlations, Non-equilibrium Green's Functions
PACS: 05.30.-d,05.60.Gg,72.10.Bg,73.23.-b,73.63-b

1. MOLECULAR BRIDGE IN TRANSIENT REGIME

We study electronic transients in the well-known model of molecular bridge [1] :

LEFT LEAD	J_L	BRIDGE ISLAND	J_R	RIGHT LEAD

The central island is represented by a single molecular level, while the leads are metallic and serve as both particle and energy reservoirs. They are floating at their externally imposed potentials kept at a finite bias. The connectivity in the system is controlled by the two tunelling junctions J_L and J_R. In the paper [2], we have introduced a formalism for calculating the transient response of the electrons to sudden changes of the connectivity, modelled by switching on or off each of the two junctions independently. We use the technique of time-partitioning for non-equilibrium Green's functions (NGF)whose general framework is described in [3]. For a parallel development based on NGF and the time-dependent density functional, the most recent reference is [4].

Here, we present and discuss first results of calculation of these transients, using the model of independent electrons and looking at the time dependence of the occupancy of the central island. The initial transient reflects the details of the tunneling through the junctions and depends sensitively on the initial conditions at the time of the sudden change of the connectivity. These may be simple, dependent on the one-particle distribution only, called uncorrelated (UIC), or they may be "correlated" that is incorporate higher order initial correlations (CIC). The initial transient typically dies out within a decay time $\tau^\star \cong \max\{\tau_Q, \tau_c\}$ (Q ... quasi-particle formation, c ... decay of correlations). The generic quasi-particle (QP) stage ensues characterized by a relaxation time $\tau \gg \tau^\star$.

2. FORMAL TREATMENT AND RESULTS

The central island occupancy for $t > t_{\mathrm{I}}$, where the initial time t_{I} coincides with the switching time of a junction, has the following NGF form:

$$n(t) = G^R(t,t_{\mathrm{I}})n(t_{\mathrm{I}})G^A(t_{\mathrm{I}},t) - \mathrm{i}\int_{t_{\mathrm{I}}}^{t}\mathrm{d}v\int_{t_{\mathrm{I}}}^{t}\mathrm{d}u\, G^R(t,v)(\Sigma^<(v,u) + \{\text{CIC terms}\})G^A(u,t) \tag{1}$$

It has the first, coherent transient, term and the integral "transport term", persisting in time. The time range of the $\Sigma^<$ self-energy is τ_c. These two terms together reflect the UIC. The additional CIC terms have kernels acting within a $\sim\tau_c$ vicinity of t_{I}. They express the initial correlations in terms of their gradual build-up during the bridge history prior to t_{I}. Propagators $G^{R,A}$ have a QP formation period $\sim\tau_Q$ followed by the standard QP regime.

The results in Fig.1 are for a semirealistic model with leads of heavily doped semiconductor at nitrogen temperature. The island starts as disconnected, with the level occupancy $n = 1$. First, at $t_{\mathrm{I}} = 0\,$fs, J_L is switched on. We see the UIC controlled transient given mostly by the QP formation. A saturation tending to $n \sim 0.78$ follows. This is interrupted by connecting also J_R at $t_{\mathrm{I}} = 25\,$fs. The transient starts now from a correlated initial state. To show the effect of CIC, we also plot the transient with correlations neglected, largely repeating the J_L behavior before. Again, the gradual saturation, now to $n = 0.51$ follows. The initial correlations decay quickly, but their cummulative effect is propagated by $G^{R,A}$ with the damping time equal to the QP relaxation time.

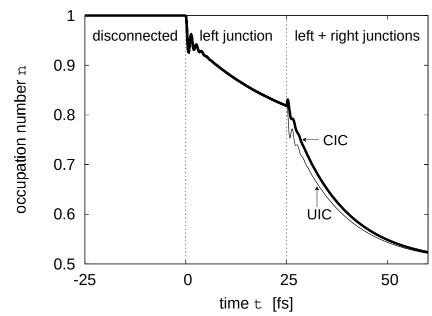

FIGURE 1. Island occupation number. For $-25 < t < 0$ ("disconnected") J_L, J_R are off. For $0 < t < 25$ ("left junction") J_L is on, J_R is off ... UIC transient. For $25 < t$ ("left+right junction") both J_L, J_R are on ... CIC transient. An artificial UIC transient is show for comparison, see curve labels.

ACKNOWLEDGMENTS

This research was partially supported by the Grant Agency of the Czech Republic within the grant project 202/08/0361. The research was carried out by A.K. within the Institutional Research Plan AV0Z10100520, by V.S. within the AVOZ10100521, both financed by the Academy of Sciences of the Czech Republic and by B.V. within MSM0021620845 financed by the Ministry of Education.

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