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Non-equilibrium dynamics of open quantum systems Limits to simplified description by Generalized Master Equations

The talk will deal with problems of a proper description of electron dynamics of open quantum systems when initial conditions, quantum interferences and decoherence processes play important roles. The aim is to understand the full time development of many-body open systems out of equilibrium from its initial state over its transient dynamics to its very long time dynamics. After the disturbances cease acting and the initial correlations die out, the process can enter the non-equilibrium quasi-particle mode permitting, under some circumstances, a reduced description. The possibility of simplified descriptions will be demonstrated on non-equilibrium dynamics of the molecular bridge model represented by calculations of transient magnetic currents between two ferromagnetic electrodes linked by tunneling junctions to a molecular size island of an Anderson local center type. The model can be treated using the non-equilibrium Greens functions (NGF) [1] numerically. This provides a reference framework for testing the possibility of a simpler solution by a Generalized Master Equation resulting from the NGF scheme approximated by the Generalized Kadanoff - Baym Ansatz (GKBA) [1, 2]. It turns out that the decisive feature is the spectral structure of the tunneling functions of both electrodes and their positioning with respect to the island level depending on the bias and the exchange splitting. Favorable for the validity of an Ansatz are weak tunneling and spectrally flat tunneling functions [2,3].

[1] V. Špička, A. Kalvová, B. Velický, Int. J. Mod. Phys. B 28, 1430013 (2014). [2] A. Kalvová, V. Špička and B. Velický, J. Supercond. and Novel Mag., DOI 10.1007/s10948-016-3680-2 (2016). [3] V. Špička, A. Kalvová, B. Velický, Fortschritte der Physik, to be published (2017) .

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