Dynamics of open systems, fluctuation-dissipation theorems and quantum transport theory

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This talk will deal with the problem of the proper description of electron dynamics of open quantum systems out of equilibrium from a finite time initial state over the transient period to the long time asymptotic.

The formulation of a simplified transport theory of non-equilibrium dynamics of electrons in quantum systems, based on the Fluctuation-Dissipation (FD) theorem, will be addressed. The FD theorem will be formulated within the Non-Equilibrium Green Function (NEGF) formalism. The relation of the simplified Generalized Master Equation (GME) description to non-equilibrium generalization of FDT will be shown independently on the chosen model.

The possibility of such a simplified description will be first discussed 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. This model can be treated by using the full set of equations for NEGF, which can be solved numerically.

This provides a reference framework for testing the possibility of a simpler and physically more transparent solution based on a Non-Markovian GME as an approximation of the full set of NEGF equations, which can be derived by using the Generalized Kadanoff-Baym Ansatz (GKBA) [1,2]. The limitations and possible improvements of the GKBA type of approximations, as well as an improved GME, based on the use of a corrected GKBA, will be discussed [2,3].

[1] V. Špička, A. Kalvová, B. Velický, Int. J. Mod. Phys B 28, 1430013 (2014).

[2] V. Špička, A. Kalvová, B. Velický, Fortschritte der Physik 65 17 00032 (2017).

[3] A. Kalvová, B. Velický, V. Špička, EPL 121, 67002 (2018).