Relation between full NEGF, Non-Markovian and Markovian transport equations

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This contribution addresses the problem of a proper description of electron dynamics of small open quantum systems out of equilibrium from a finite time initial state over the transient period to the long time asymptotics.

The standard tool, Non-Equilibrium Green's Functions (NEGF), can well be simplified, under some conditions, to Non-Markovian Generalized Master Equations (GME) for single particle density. The conventional approximation for this purpose, based on the causal Generalized Kadanoff-Baym Ansatz (GKBA), has been fairly succesful in practice, but exact criteria for its validity are missing so far.

This problem may be attacked for a variant of the generic molecular island model, an Anderson impurity linked between two bulk metallic leads by tunneling junctions: our electrodes are ferromagnetic, so that transient currents are spin polarized and the tunneling functions have a complex spectral structure. The transient studied is a free relaxation of an initial state created by suddenly switching on of both junctions.

In the first step, explicit conditions are obtained for the use of GKBA, permitting to delimit the range for reducing NEGF to a GME. In the second step, an asymptotic approximation for the vertex corrections to GKBA is proposed. This leads to a renormalized GME with a substantially extended applicability range. Implications for further reduction to a Markovian Master Equation are indicated.

Finally, the relation of the GME description to possible non-equilibrium generalizations of the Fluctuation-Dissipation Theorem (NE FDT) is shown, extended beyond the present model within the NEGF formalism and physically interpreted in terms of a simplified kinetic theory of non equilibrium electrons in open quantum systems.