

Applying time-local quantum master equations to dissipative dynamics and transport

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This talk focuses on the description of molecular quantum dynamics in complex environments. The dynamics in so-called open quantum systems is often described by quantum master equations. After briefly reviewing the theoretical background of the approach and its recent extensions, several different systems will be discussed. In the first type of applications the environment will consist of a thermal bath. As an application we will focus on describing the energy transfer dynamics in light-harvesting systems of purple bacteria with parameters stemming from molecular dynamics and quantum chemical simulations. In contrast the environment can also describe fermionic particle reservoirs and as a prime example we will discuss the charge transfer in molecular wires. Here a special emphasis will be put on time-dependent effects.

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