

22nd of July, 2025 – 11:00
 CFEL – Building 99, seminar room I (ground floor)

Frank Großmann



from Technical University, Dresden (Germany)

***Non-Markovianity in open quantum systems:
 From vibrational relaxation at surfaces
 to adiabatic population transfer***

We review the multi Davydov-Ansatz for the solution of the time-dependent Schrödinger equation of a multi-level system coupled to a (finite) bath of harmonic oscillator modes and compare its performance to the HOPS method [1]. Two novel applications of the Davydov-method will then be highlighted:

(i) Firstly, we investigated the vibrational relaxation dynamics at surfaces focussing on the D-Si-Si bending mode at a D:Si(100)-(2x1) surface.

Here a hierarchical effective mode model [2] allows to effectively treat a bath of more than 2000 phonon modes. Non-Markovianity is quantified by a comparison to a Lindblad-type Liouville von Neumann approach [3].

(ii) Secondly, a stabilization of the transition probability from the lower to the upper level as a function of the area under the laser pulse in the case of rapid adiabatic passage in a two-level setup was found [4]. This dissipative engineering effect could only be uncovered by an intrinsically non-Markovian treatment. For strong coupling, the transition probability then becomes a monotonically increasing function of the pulse area at zero temperature of the heat bath. Finite temperatures break the monotonicity in the range of pulse areas that we studied but not the stability of the observed effect.

[1] R. Hartmann, M. Werther, F. Grossmann and W. T. Strunz, J. Chem. Phys. 150, 234105 (2019)

[2] E. W. Fischer et al, J. Chem. Phys. 153 064704 (2020)

[3] E. W. Fischer et al, J. Chem. Phys. 156 214702 (2022)

[4] M. Werther and F. Grossmann, Phys. Rev. A 102, 063710 (2020)