

# Seminar on Condensed Matter Theory

Group of Theoretical Physics at the Department of Condensed Matter Physics  
of Charles University has a pleasure to invite you to attend the seminar

**on 28 May 2019 at 13:00**

at Faculty of Mathematics and Physics of Charles University, Ke Karlovu 5, 121 16 Praha 2

**Seminar room F052**



## M.Sc. Christoph Kaspar

*University of Freiburg, Germany*

### Influence of nonadiabatic electronic-vibrational effects on the quantum transport through single-molecule junctions

Note special day and time.

The coupling of electronic and nuclear degrees of freedom is an important mechanism in non-equilibrium charge transport in molecular junctions and may result in a variety of interesting phenomena such as decoherence, switching and local cooling or heating [1]. While the effect of adiabatic polaron-type coupling has been studied in great detail, new phenomena are expected for non-adiabatic coupling scenarios which correspond to a breakdown of the Born-Oppenheimer approximation. In this contribution, we present results of a model study of non-adiabatic effects employing the hierarchical quantum master equation approach [2,3]. This method generalizes perturbative master equation methods by including higher-order contributions as well as non-Markovian memory and allows for the systematic convergence of results. In particular, we observe a quantum transport behavior strongly influenced by the interaction with the vibrational modes. Assuming the scenario of two degenerate electronic states coupled to two degenerate vibrational modes leads to new interesting phenomena [4].

[1] Härtle et al., Phys. Rev. B 98, 081404 (2018)

[2] Jin et al., J. Chem. Phys. 128, 234703 (2008)

[3] Schinabeck et al., Phys. Rev. B 94, 201407R (2016)

[4] Schultz et al. Phys. Rev. B 77, 0753223 (2008)

