Graduate School Seminar

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AG Molecular Quantum Dynamics

Dissipative exciton dynamics in light-harvesting complexes – developing methods and models to understand a primary step of photosynthesis

Photosynthesis, that is the conversion of sunlight into chemical energy, by algae, bacteria, and plants is the main energy harvesting mechanism on earth. The general scheme of this process is well understood. Light is absorbed by specialized so-called light-harvesting antenna complexes. Thereby Frenkel excitons are formed which can be transferred through linker aggregates to reaction centers, where charge separation processes occur. The charge separation leads to chemical potentials which drive the main chemical reactions like the synthesis of sugars.
The nature of the energy transfer and especially the optimization mechanisms applied by nature are still not fully understood although investigated for nearly a century. It was suggested early that there appears an incoherent “hopping” of the excitons (Förster type transfer). However, recent experimental results suggested that quantum coherence might play an important role. In order to study the exciton transport in light-harvesting antennae quantum-mechanically a system-bath separation is required to include both, the electronic and vibrational degrees of freedom of the system.
The talk will introduce the basic models to mimic molecular aggregates embedded in an environment and the Hierarchy Equations of Motion (HEOM) method which is applied to calculate the dissipative exciton dynamics and spectra. HEOM provides a powerful tool for investigations as it is an in principle exact method and can be applied to rather large systems. Further, preliminary results concerning the influence of quantum state mixing on the dynamics in small aggregates will be presented.

Talk: English
Slides: English

Location: Institute of Physics, Albert-Einstein-Str. 24, HS1

Talks in WS 2015/16

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