Physikalisches Institut
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Quantum Efficiency
Seminar und Colloquium

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Coherent and Incoherent Energy Transfer in Light-Harvesting Systems

Excitonic energy transfer from light harvesting complexes towards the photosynthetic reaction center constitutes a crucial ingredient for the conversion of light into chemical energy. From a dynamical point of view it consists of a sequence of exciton transfer steps along a network of chromophores. Despite the high temperatures at which photosynthesis typically takes place, recent experimental findings suggest the existence of coherent dynamics in these processes, which might help to understand the surprisingly high efficiency with which captured light is funneled into the reaction center to fuel the charge separation.

Sparked by these exciting reports, a variety of different theoretical approaches has been unsed to study the microscopic dynamics of this energy transfer in the framework of dissipative tight-binding models. Among them are path integral Monte Carlo (PIMC) simulations, which offer the advantages of being numerically exact as well as capable to deal with arbitrary spectral densities of the various environmental degrees of freedom, summarizing the protein scaffold as well as residual water molecules. The flexibility of this approach allows to explore both the case of correlated as well as uncorrelated environments with respect to the individual chromophores and their influence on the coherent-incoherent transition. Utilizing spectral densities obtained from recent MD and mixed quantum-chemical studies [1,2] we can further give a detailed account of excitonic energy transfer in the FMO complex at room temperature, revealing, e.g., the importance of preparational effects on the visibility of coherent excitonic motion [3]. Finally, combining the PIMC approach and Lindblad calculations, the exact PIMC results can be extrapolated to, in principle, arbitrarily long times [4], thus giving access to experimentally measured quantities like absorption spectra.

[1] Carsten Olbrich, Johan Strümpfer, Klaus Schulten, and Ulrich Kleinekathöfer, JPCL, 2, 1771 (2011).
[2] Sangwoo Shim, Patrick Rebentrost, Stéphanie Valleau, and Alán Aspuru-Guzik, Biophys. J. 102, 649 (2012).
[3] Lothar Mühlbacher and Ulrich Kleinekathöfer, JPCB 116, 3900 (2012).
[4] Oliver Mülken, Lothar Mühlbacher, Tobias Schmid, and Alexander Blumen, PRE 81, 041114 (2010).

Date:	**Tuesday, October 30th, 2012 14:15 pm**
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