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Coherence and energy transport in molecular aggregates: stochastic approach[1] DARIUS ABRAMAVICIUS, VYTAUTAS ABRAMAVICIUS, VLADIMIR CHOROSAJEV, Theoretical Physics Department, Vilnius University — Recent spectroscopy studies of various molecular assemblies have shown that optically induced quantum coherences in these systems survive much longer than predicted from standard rate equations. This result sparked numerous debates whether the coherent system dynamics are related to the efficiency and/or speed of the excitation energy transfer in such systems. The problem could be addressed by studying coherent excitation dynamics and its relaxation due to interaction with the bath. The reduced density matrix propagation theories provide the reduced/averaged information on the dynamics. Stochastic approaches allow accessing more detailed microscopic picture. Two types of stochastic equations have been derived for a system coupled to the bath of an arbitrary spectral density. The stochastic wave functions allowed to define excitation coherent dynamics, polaron formation dynamics and energy relaxation times together with energy transport pathways in molecular aggregates. Simulations of the energy transport in few model molecular aggregates were performed using both approaches for the system wavefunction. It was demonstrated that the quantum coherences in the system appearing from mixture of vibrational and excitonic resonances significantly affect the energy transport process.

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