Excitation energy transport in biological and structured environments: a time-adaptive density matrix renormalization group approach

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Abstract

Recent ultra-fast optical experiments on photosynthetic pigment-protein complexes (PPC) have observed surprisingly long-lasting electronic coherences which can persist right up to room temperature. These previously unexpected coherences have been found in structures which are responsible for an essentially lossless transport of solar energy to reaction centers where the energy is used to initiate photosynthetic chemistry. It has now been suggested that quantum coherence may play a key role in achieving this efficient and biologically crucial transport, and in this talk I will discuss a number of mechanisms by which coherence and dissipative dynamics can conspire to drive lossless transport in PPC structures. A key feature of these systems is the strong coupling to the slow local protein environments, environments with correlation times which may be easily comparable to the dynamical timescales of the excitations. In order to explore the realistic and highly non-markovian excitation dynamics of PPCs, we perform many-body simulations of the system and environment using the time-adaptive renormalization group method (t-DMRG). This technique allows us to obtain extremely accurate dynamics for impurities coupled to arbitrarily complex spectral functions, and results for several spectral functions of relevance to PPCs will be presented. This method also allows the simulation of ground states of impurities in strong interaction with their environments, and, if time permits, some results on the ground state of the sub-Ohmic spin boson will be presented and discussed.