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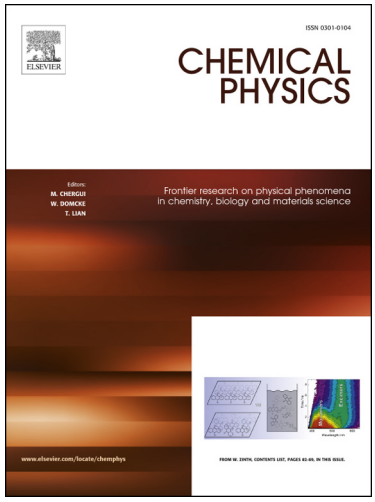

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Dynamic Coherence in Excitonic Molecular Complexes under Various Excitation Conditions

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Abstract

We investigate the relevance of dynamic quantum coherence in the energy transfer efficiency of molecular aggregates. We derive the time evolution of the density matrix for an open quantum system excited by light or by a neighboring antenna. Unlike in the classical case, the quantum description does not allow for a formal decomposition of the dynamics into sudden jumps in an observable quantity – an expectation value. Rather, there is a natural finite time-scale associated with the excitation process. We propose a simple experiment to test the influence of this time scale on the yield of photosynthesis. We demonstrate, using typical parameters of the Fenna-Matthews-Olson (FMO) complex and a typical energy transfer rate from the chlorosome baseplate, that dynamic coherences are averaged out in the complex even when the FMO model is completely free of all dissipation and dephasing.

Keywords: classical *vs* quantum ensemble average, quantum jumps, incoherent excitation, dynamic quantum coherence, excitonic energy transfer.

1. Introduction

Electronic excited state delocalization has been since long known to play a significant role in establishing the energy transport properties of the light-harvesting complexes (LHC) of both plants and bacteria and molecular aggregates in general (e.g. [1, 2, 3, 4]). Delocalization of the electronic eigenstates over more than one pigment corresponds to a correlation between electrons of different pigments in the same molecular crystal or aggregate which results from their direct mutual electrostatic interaction. Correspondingly, this effect has been often referred to as *electronic quantum coherence.* In photosynthetic antennae, the excited eigenstate delocalization enables fast (sub ps) transfer of excitation in space and, in combination with the influence of the virtually infinite number of degrees of freedom (DOF) of the protein environment, it directs

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