Partial Linearized Density Matrix (PLDM) Dynamics Study of Excitation Energy Transfer in Photosystem II

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The recently developed Partial Linearized Density Matrix (PLDM) propagation method [P. Huo and D.F. Coker J. Chem. Phys. **135**, 201101 (2011)] is used to explore excitation energy transfer in an extended model of Photo System II, including both energy transfer inside the CP47 - CP43 complex, and between CP47 and the reaction center (RC). The model studies also include couplings that describe the conversion between exciton and charge transfer states inside the RC, so the complete light harvesting - energy transfer and transduction process can be explored from a fully quantum dynamical perspective. We find that though the exciton dynamics inside the sub-complex occurs coherently and involves population beating between different single exciton states involving different chromophores, the total energy transfer rate determining step that involves inter sub-unit excitation transfer from chromophores in CP47 to others in the RC, occurs incoherently. Moreover, when the special pair in the reaction center is excited by these energy transfer processes, different CT states can be generated and our model calculations suggest that the Phe1- P1+ state is the predominant charge transfer state resulting after 10 ps in good agreement with the recent experiment findings.