

Abstract Submitted
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Modeling Exciton Transport in the Photosystem II Reaction Center via the Modified Generalized Quantum Master Equation KRISTINA LENN, ELLEN MULVIHILL, XING GAO, University of Michigan, ALEXANDER SCHUBERT, University of Jena, EITAN GEVA, University of Michigan — Organic solar cell materials are a cheaper option to traditional silicon but lack the efficiency for which silicon is famous. Quantum computers can outperform the greatest supercomputer, but the short-lived coherences lead to classical-like behavior. Light-harvesting systems (LHS) serve as an example to both applications. LHSs absorb sunlight and convert it into an electrochemical gradient with near unity quantum efficiency and maintain long coherence times. Probing the exciton dynamics of these systems, one of which is the Photosystem II reaction center (PSII RC), can elucidate how these systems are able to transport excitons with approximately 99% efficiency. To do this, we have employed a projection-free version of the Generalized Quantum Master Equation (GQME) whose memory kernel is calculated using approximate methods, such as the Mean-Field Approximation (MFA) and the Linearized Semiclassical Method (LSC). This approach, verified against a Spin-Boson model and the well-studied LHS Fenna-Matthews-Olson (FMO) complex, is more computationally efficient and yields a high level of accuracy compared to exact methods such as the Quasi-Adiabatic Propagator Path Integral (QuAPI).

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