Coherent Energy Transfer in Light-harvesting: Symmetry, Disorder, and Noise

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Quantum coherence plays a central role in natural and artificial light-harvesting complexes and is explored by my group in terms of symmetry, static disorder, and the size and alignment of these complexes.

(1) An intriguing observation of photosynthetic light-harvesting systems is the N-fold symmetry of light-harvesting complex 2 (LH2) of purple bacteria. We have calculated the optimal rotational configuration of N-fold rings on a hexagonal lattice, and established the symmetry principles for the promotion of maximum excitation energy transfer (EET). For certain fold numbers, there exist optimal basis cells with rotational symmetry, extendable to the entire hexagonal lattice for the global optimization of the EET network, such that these basis cells can reduce or remove the frustration of EET rates across the photosynthetic network. [1] Remarkably, one consecutive group of such symmetry numbers consists of the naturally occurring 8-, 9- & 10-fold rings, suggesting the design principle of matching the internal symmetry with the lattice order.

(2) We have studied coherent quantum transport in disordered 1-D and 2-D systems and clearly showed an optimal diffusion constant at an intermediate level of noise. [2] Scaling analysis similar to the mean first passage time analysis [3] indicates the crucial role of localization length. Further detailed studies reveal that optimal diffusion depends critically on dimensionality and range of interactions, and may not be observed in certain systems due to different scaling laws. We are also developing methods to calculate transport in a thermal environment and predict its temperature-dependence.

(3) We have developed a novel numerical method [4] to predict the quantum dynamics of extended systems. Based on the concept of dynamical maps, our method extracts all available information encapsulated in short-time non-Markovian quantum trajectories and compresses it into tensors of reduced size. Efficient propagation of these tensors generates dissipative quantum dynamics of large systems with arbitrary spectral densities, e.g., molecular chains of hundreds of sites with strong quantum dissipation. Further, it can be applied to experimental settings in the same spirit as processing tomography and permits direct reconstruction of dynamical operators, i.e., the Hamitonian and memory kernel.

[1] Cleary, Chen, Chern, Silbey, and Cao, PNAS 110, p8537 (2013)

[2] Jeremy, Khasin, Cao, New Journal of Physics 15, 085010 (2013)

[3] Wu, Silbey, and Cao, PRL 110, p200402 (2013)

[4] Cerrillo and Cao, PRL accepted (2014)