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Using linear spectroscopy to accurately determine the Hamiltonian of a light-harvesting complex

Linear optical spectroscopy is a crucial analytical tool in biology, chemistry, materials science, molecular physics, and various other disciplines, but is hard to simulate exactly—even for small model systems. In this presentation we give an overview of different linear spectroscopy techniques and briefly discuss approximate methods and an exact method for the calculation of linear spectra. We also investigate the validity of the approximate methods by comparing their spectra to the exact spectra of a dimer. We apply the best method in a spectral fitting procedure, called Particle Swarm Optimization (PSO), to determine the Hamiltonian of the light-harvesting complex CP29 of plants. The latter is thought to act as a conduit, and perhaps energy switch, for excitation energy collected by the plant's photosynthetic antenna apparatus. Using our calculated Hamiltonian for CP29, we model excitation energy flow through this complex and discuss its possible roles in the harvesting of light by plants.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

Consent on use of personal information: Abstract Submission

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