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Modelling linear spectra of plant light-harvesting complexes

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During the initial stage of photosynthesis, sunlight is absorbed by molecular light-harvesting complexes. The technique of linear optical spectroscopy is a powerful tool to study these complexes. In principle, all the information contained in an experimental linear spectrum can be extracted through comparison with the corresponding modelled spectrum—provided that the modelling is accurate. In this presentation, we discuss the physics underlying linear spectroscopy and how these spectra can be modelled. We consider an exact method based on stochastic path integration (PI) and several approximate methods, including the Full Cumulant Expansion (FCE), complex time-dependent Redfield (ctR), Redfield, and modified Redfield methods. We characterize the accuracy of the approximate methods for modelling absorption- and fluorescence-type linear spectra by comparing the approximate spectra with exact spectra for a model system similar to plant light-harvesting complexes. We show that the FCE method performs best for absorption-type spectra but, surprisingly, may break down when calculating fluorescence-type spectra. We also show that the often-used Redfield and modified Redfield methods both perform poorly. We consider two applications of linear spectral modelling. First, we use particle swarm optimisation (PSO) to fit the experimental spectra of the plant light-harvesting complex CP29 with modelled spectra. Based on the molecular parameters producing the best fit, we show that CP29 likely has a dual role as an excitation conduit and as a dissipater of excess energy. As a second application of spectral modelling, we train neural networks to predict disordered linear spectra from molecular parameters and *vice versa*. We show that the neural network models can make accurate predictions orders of magnitude faster than the traditional modelling methods.

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

Yes

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

PhD

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