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Applications of machine learning techniques to the description of quantum coherent excitation energy transfer within the dimer model

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During photosynthesis in light-harvesting complexes, energy is transferred from antenna pigments to the reaction centre to trigger photochemical reactions. The idea of quantum coherence playing a role in photosynthesis arose from observations that excitation energy transfer (EET) processes in these complexes are efficient to an extent that exceeds explanation using only classical theory. The formalism adopted to study EET processes is the Hierarchical Equations of Motion (HEOM). However, solving these equations is computationally costly due to the adverse scaling with the number of pigments. We use a trained convolutional neural network as a representation of the HEOM where elements of reduced density matrices are translated into features for the model and corresponding excited state energies and electronic couplings are used as labels. We discuss the investigation of the spin-boson-type model where our predictions of the parameters for the Frenkel Hamiltonian are gauged by mean square error and accuracy measures.

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