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A Tuneable Framework for Vibronic Dynamics: Generalized Nonlinear Exciton Equations

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Accurately modeling coupled electronic–vibrational dynamics in molecular aggregates is essential for interpreting energy transfer and nonlinear optical signals. We present a non-perturbative framework based on Generalized Nonlinear Exciton Equations (NEE) derived from the Heisenberg equation for a Frenkel-exciton Hamiltonian. A central feature is a generalized commutation scheme introducing a single parameter η that continuously interpolates between bosonic and paulionic statistics, enabling flexible descriptions beyond either limit. The formalism rigorously treats a linearly coupled harmonic bath, yielding a closed hierarchy for exciton populations or coherences and mixed exciton–phonon correlations.

We position two practical closures within this hierarchy. First, the Mean-Field Approximation (MFA)—a full factorization of exciton–phonon averages—recovers a limit in which quantum excitons evolve in an effectively classical bath; we quantify regimes where MFA is accurate and where it breaks down. Second, the 1-Quantum Approximation (1QA) retains only single-quantum vibrational excitations and the leading exciton–phonon coherences; we use 1QA as a controlled reduction that preserves vibronic resonances at moderate cost.

As an application, we provide preliminaries for the bacterial reaction center (BRC): site-based Hamiltonian construction for the special pair and accessory pigments and the transition-dipole orientations taken from structure.

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