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COHERENT ENERGY AND CHARGE TRANSPORT IN MOLECULAR SYSTEMS

2. Non-Markovian System-Environment Interactions

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Abstract:

As illustrated in Lecture 1, non-Markovian behavior is ubiquitous in molecular systems. Here, we address three different approaches which are adapted to a quantum-dynamical description in such markedly non-Markovian situations. The first approach relies on explicit high-dimensional simulations of the combined molecule-plus-environment system, with a discretized representation of the environment. The second approach relates to non-Markovian master equations, employing local and non-local-in-time variants. The third approach interpolates between the first two schemes, in that a subset of effective environmental modes are treated explicitly, while the residual environment is included in a master equation setting. Typical examples are given for these three approaches, illustrating the role of coherence and correlations.