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Quantum dynamics of phonon-limited charge and energy transport: Numerically exact and approximate approaches

Recent interest in quantum dynamics of electronic excitations in molecular semiconductors and photosynthetic molecular aggregates [1] is motivated by the prospect of optoelectronic applications that could harness quantum effects and enhance charge and energy transport. Typically, the coupling of charges or excitons to quantum lattice vibrations lies in the intermediate regime, whose reasonable description necessitates computationally expensive numerically exact approaches. Meanwhile, coupled electronic–vibrational dynamics occurring on a wide range of timescales is inaccessible to most existing methods, suggesting a need for new (approximate) approaches.
In this talk, I give a synthetic overview of my recent methodological breakthroughs [2–4] concerning electronic quantum dynamics in the field of phonons.
I present the applications of the numerically exact hierarchical equations of motion (HEOM) method to the Holstein [2] and Peierls models [3]. I discuss how to overcome the method's numerical instabilities stemming from strong non-Markovian effects [2] and handle the phonon-assisted current in the Peierls model [3]. These developments enable us to answer long-standing questions such as the importance of vertex corrections to conductivity in the Holstein model [2] or the appropriateness of the transient localization scenario for charge transport in the Peierls model [3]. Finally, I show how the synergy between the theory of open quantum systems and diagrammatics of condensed matter physics can be used to devise an approximate approach to exciton dynamics in multichromophoric aggregates [4]. I discuss the application to laser-triggered exciton dynamics the Fenna–Matthews–Olson complex immersed in a realistic structured bosonic environment.

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[4] V. Jankovic and T. Mancal, J. Chem. Phys. 161, 204108 (2024).

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