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Real-time quantum electron-phonon dynamics[1] VALERIO RIZZI, TCHAVDAR TODOROV, JORGE KOHANOFF, Queen's University Belfast, ALFREDO CORREA, Lawrence Livermore National Laboratory — Electrons and atomic motion out of equilibrium exchange energy and momentum. Physical problems that involve this exchange include Joule heating, inelastic electron tunneling, and thermalization of hot electrons in an irradiated material. An explicit dynamical treatment of both subsystems is essential to model such non-adiabatic phenomena and requires the ability to describe the interaction of the coupled electrons and nuclei without enforcing equilibration *a priori*. Therefore, being able to describe an electronic system in real time together with the underlying ionic system is a key feature for first-principles electron-phonon methods. We have developed an approach for real-time phonon-assisted electron transfer in nanowires, explicitly tracking out-of-equilibrium systems that exchange energy. Our model is fully quantum mechanical: it overcomes the limitations of the Ehrenfest (quantum-classical) approximation and doesn't require thermostats, or the treatment of either subsystem as a bath. We can probe a range of timescales: from attoseconds (electronic timescale) to picoseconds (typical of atomic vibrations). The comparison with exact simulations of systems with a single phonon and a single electron have proved an invaluable validation tool for our method. We are able to describe the population inversion of an excited electronic system coupled to phonons and phonon-assisted conduction in systems with Anderson localization.

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