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Real-Time Path Integral Study of Electron Transport in Molecular Wires: A Constant Current Formulation and the Importance of Dissipative Processes ROBERTO LAMBERT, KE DONG, NANCY MAKRI, University of Illinois at Urbana-Champaign — We report the results of real-time path integral calculations to study electron transport in molecular-wire models. The molecular wire system is modeled by a multi-site one-electron tight-binding Hamiltonian connected to two metal electrodes and coupled to a bath mimicking the dissipative effects of molecular vibrations. In order to maintain a steady current flow, we introduce a simple recharging model in which electrons are injected from the donor electron as needed to replenish charge lost to the acceptor, maintaining a constant electron population within the wire. Using real-time path-integral techniques, we study the conductance of the molecular wire model as a function of wire length, with emphasis on the effects of its dependence on dissipation.

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