Abstract Submitted
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The spectroscopic dynamics of electron transport through molecular junctions ALEXANDER PROCIUK, BARRY DUNIETZ, University of Michigan — A non-equilibrium Green's-Function (NEGF) model based on time dependent perturbation theory is developed to compute the spectroscopic dynamics of electron transport through molecular junctions under the influence of weak time dependent classical fields. In this model, we use the two time variable nature of the Kadanoff-Baym equations of motion to formulate a mixed time-frequency representation for the electronic density. The resulting highly informative time dependent Wigner distributions are used to shed light on the features of dynamical observables, such as electron current, dipole moment and population. We analyze laser induced coherence and population transfer effects for both Markovian and non-Markovian electrode models. If time permits, the analysis of transient conductance with respect to the system's fundamental parameters will be discussed.

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