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Time-Dependent Transport Phenomena: Bound-State Oscillations and Pumping STEFAN KURTH, ELHAM KHOSRAVI, Institute for Theoretical Physics, Free University Berlin, Berlin, Germany, GIANLUCA STEFANUCCI, University of Rome Tor Vergata, Rome, Italy, ANGEL RUBIO, University of the Basque Country and Donostia International Physics Center, San Sebastian, Spain, EBERHARD K.U. GROSS, Institute for Theoretical Physics, Free University Berlin, Berlin, Germany — We present a description of transport based on the time evolution of the non-interacting time-dependent Schrödinger equation and develop a numerical algorithm for the time propagation which is suited for implementation of time-dependent density functional theory (TDDFT). The algorithm is used to study time-dependent transport phenomena such as electron pumping, transients and bound state oscillations. It has been shown recently [Phys. Rev. B **75**, 195115 (2007)] that the presence of at least two bound states in the biased electrode-device-electrode system of non interacting electrons leads to persistent oscillations in the total current whose amplitude depends on the history of the applied voltage and on the initial state. In the case of electron pumps driven by time-periodic gate voltages, the amplitude of these oscillations decays slowly with time. TDDFT results will be compared to those obtained for non-interacting electrons.

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