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Non-steady state in quantum transport ELHAM KHOSRAVI, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany, STEFAN KURTH, Nano-Bio Spectroscopy Group, Departamento de Fisica de Materiales, Universidad del Pais Vasco, Avenida de Tolosa 72, E-20018 San Sebastian, Spain, GIANLUCA STEFANUCCI, Dipartimento di Fisica, Universita di Roma Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy, E.K.U. GROSS, Max Planck Institute of Microstructure Physics, Weinberg 2, D - 06120 Halle, Germany — The standard approach to quantum transport combines the Landauer-Buettiker (LB) formalism with ground-state density functional theory (DFT). The basic assumption of this approach is that a steady state is achieved after turning on a DC bias. Here we show that this assumption is "not" valid in general and and give examples for which no steady state develop within several adiabatic (time-local) approximations as well as in non-interacting systems. In these cases a time-dependent description of transport is essential. For the non-interacting case, the presence of bound states in a biased system is shown analytically and numerically to lead to persistent, localized current oscillations which can be much larger than the steady part of the current (PCCP. 11, 4535(2009)). For the interacting case, the discontinuity of the exchange-correlation potential of DFT in the context of electron transport for an interacting nanojunction attached to biased leads, gives rise to a dynamical state characterized by correlation-induced current oscillations in the Coulomb-blockade regime (PRL. 104, 236801(2010)). In addition, for multistable systems, the time-dependent approach describes if and how a solution can be reached through time evolution.

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