

Abstract Submitted
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Time-dependent NEGF calculations of extended systems

ALEXANDER PROCIUK, BARRY DUNIETZ, University of Michigan — A non-equilibrium GF (NEGF) model based on time dependent perturbation theory is developed to propagate electronic structure and molecular conductance of extended electrode-molecule-electrode nanostructures. In this model, we take advantage of the two time variable nature of the KB equations in order to formulate a mixed time-frequency representation for the lesser GF. This allows us to include bulk affected electrodes with non-trivial energy representations in our propagation. It also allows us to express dynamical observables such as current with highly informative Wigner distributions that shed light on the physical causes for certain dynamic features. Preliminary calculations, performed on simple systems, reveal that the dynamic current has both a direct and an alternating contribution. The direct current is due to a bulk affected state and the alternating component is due to a superposition of states. The amplitude of the alternating current can be changed dramatically by adjusting the bias pulse.

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